**Book Chapter**

**Effect of Electronegativity on Structural, Spectrophotometric and Thermo-Chemical Properties of Fluorine and Chlorine Substituted Isoxazoles by DFT Method**

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Abstract

The effect of electronegativity (F and Cl atom) on structural, spectrophotometric, thermo-chemical properties, and solvent effect on electronic absorption spectra of \{3-(3,5-dichloro-2-hydroxyphenyl)-5-[(4-fluorophenyl)amino] isoxazol-4-yl\}(phenyl)methanone (Ia) and \{3-(3,5-dichloro-2-hydroxyphenyl)-5-[(4-chlorophenyl)amino] isoxazol-4-yl\}(phenyl) methanone (Ib) were studied by DFT method using PBE1PBE functional with 6-311++g (d, p) basis set. The results show that the electronegativity of halogen group affect the bond length, atomic charges, excited wavelength, molecular orbital energy gap, vibration frequency, thermo-chemical parameters, and stability of compounds.

Keywords

DFT, Electronegativity, Stability, HOMO–LUMO Gap

Public Interest Statement

The work presented here shows how computational methods used for understanding the molecular problem more clearly and that helps to design the drug with better action. In particular, the results presented here demonstrate that the DFT method is good tool for studying the stability of isoxazole by computational technique. This is a very useful tool for synthesizing a target molecule because a single compound may generate toxic waste, require months of labor, and raw materials cost. So before synthesizing the drug, firstly design the molecule, understand the molecular properties by computational method, and minimize the chemical pollution by synthesizing lots of unusable drug.
Introduction

Isoxazole derivatives are five-member nitrogen–oxygen-containing heterocyclic compounds that play an important role in pharmacological activities such as anti-cancer [1], anti-tuberculosis [2,3], anti-inflammatory [4], cytotoxic [5], antimicrobial [6], anti-HIV [7], anti-diabetic [8], antipsychotic [9,10], and anticonvulsant [11].

The density functional theory (DFT) is a common method to study the electronic structures that helps for understanding the drug activity of molecules. FT-IR, FT-Raman spectra, NBO, HOMO–LUMO, and thermodynamic properties of 4-chloro-3-nitro benzaldehyde [12], pycinaldehyde oxime [13] was satisfactorily analyzed by DFT. The spectral properties of heterocyclic compounds such as the valence shell photoelectron spectra, geometry optimization, X-ray, vibrational frequency analysis of purine, pyrimidine [14], heteroaromatic molecules [15], and substituted isoxazole [16,17] were studied using DFT calculation.

Thermodynamic properties (enthalpy, entropy, and Gibbs free energy) are important to understand the stability of molecule at different temperature and pressure that can easily explained using DFT (B3LYP/6-31G*) with the Gaussian 03 program [18,19].

In this work, a theoretical study of {3-(3,5-dichloro-2-hydroxyphenyl)-5-[(4-fluoro phenyl)amino]isoxazol-4-yl}(phenyl)methanone (Ia) and {3-(3,5-dichloro-2-hydroxyphenyl)-5-[(4-chlorophenyl)amino]isoxazol-4-yl}(phenyl)methanone (Ib) has been performed using DFT method in order to elucidate the effect of electronegativity on structural, spectrophotometric, and thermo-chemical properties.

Computational Details

All theoretical calculations performed with the Gaussian-03 package [20]. Full ground-state geometry optimizations and frequency were carried out at the DFT [21-25] using the
PBE1PBE functional [26,27] and the 6-311++g (d, p) basis set [28-32]. Electronic absorption spectra were computed as vertical electronic excitations from the ground state using TD-DFT [33-35] with PBE1PBE/6-311++g (d, p).

**Results and Discussion**

**Geometry Optimization**

The geometry optimization has started without symmetry constraints and after optimization; the structure converged to $C_1$ symmetrical species. The geometry was optimized in the lowest energy singlet ground state by DFT method with PBE1PBE function using 6-311++g (d, p) basis set in gas phase and the optimized structures of Ia and Ib shown in Figures 1 and 2, respectively.

![Figure 1: Optimized structure of Ia in gas phase.](image-url)
The geometry was non-planer because of strong distortion between electron cloud of three aromatic rings and isoxazole ring. The optimized geometric parameters of Ia and Ib are recorded in supplementary information Tables S1 and S2, respectively.

Bond lengths of isoxazole ring were not largely affected by electronegativity of fluorine and chlorine substituent but the bond lengths of 16O–17N, 14C–15C, and 15C–16O were slightly more in Ia than Ib. The 9O–10H bond length was important in formation of metal complexes but the difference between 9O–10H bond length in Ia and Ib was very less i.e. 0.00014 Å (Table 1).
Table 1: Bond length and NBO atomic charges of Ia and Ib.

| Type          | Bond Length (Å) | Atoms | NBO atomic charges |
|---------------|-----------------|-------|--------------------|
|               | Ia              | Ib    | Ia                 | Ib     |
| 16 O–17 N     | 1.40411         | 1.40355 | 9 O               | −0.695 | −0.694 |
| 17 N–13 C     | 1.30429         | 1.30435 | 10 H              | 0.500  | 0.500  |
| 13 C–14 C     | 1.44012         | 1.44027 | 13 C              | 0.209  | 0.208  |
| 14 C–15 C     | 1.39562         | 1.39489 | 14 C              | −0.320 | −0.318 |
| 15 C–16 O     | 1.32216         | 1.32195 | 15 C              | 0.608  | 0.607  |
| 15 C–31 N     | 1.34401         | 1.34522 | 16 O              | −0.339 | −0.338 |
| 31 N–32 H     | 1.01025         | 1.01047 | 17 N              | −0.141 | −0.139 |
| 14 C–18 C     | 1.44796         | 1.44871 | 18 C              | 0.544  | 0.545  |
| 18 C–19 O     | 1.23004         | 1.22974 | 19 O              | −0.592 | −0.591 |
| 13 C–3 C      | 1.47812         | 1.47802 | 31 N              | −0.584 | −0.584 |
| 9 O–10 H      | 0.98723         | 0.98709 | 32 H              | 0.427  | 0.428  |

Natural Bond Orbital Charges

The natural bond orbital (NBO) atomic charges have calculated in gas phase (Table 1). The atomic charge gives information about oxidation states of atoms in molecule, which gives important information for complex formation.

The carbon atoms connected to the high electronegative (F, Cl, O, and N) atoms were positive in nature. The 9O will provide the binding site for metal ion in formation of metal complex; as 9O contained the highest negative charge and the 10H contained highest positive charge.

Electronic Absorption Spectra

The electronic absorption spectra has computed as the lowest 10 vertical electronic excitations from the singlet ground state to singlet excited state using TD-DFT and the effect of solvent was simulated by IEFPCM (Table 2).
Table 2: Electronic absorption data in different solvent of Ia and Ib.

| Excited state | Gas phase | Water phase | Ethanol phase | DMSO phase |
|---------------|-----------|-------------|---------------|------------|
|               | $\lambda$ (nm) | $f$ | $\lambda$ (nm) | $f$ | $\lambda$ (nm) | $f$ | $\lambda$ (nm) | $f$ |
| Ia            |           |       |               |       |               |       |               |       |
| 1st           | 379.31    | 0.0511 | 360.56        | 0.1977 | 360.45        | 0.2000 | 361.22        | 0.2101 |
| 2nd           | 358.75    | 0.1055 | 318.13        | 0.0344 | 321.03        | 0.0328 | 320.33        | 0.0353 |
| 3rd           | 302.59    | 0.0049 | 288.12        | 0.0099 | 289.13        | 0.0091 | 289.02        | 0.0106 |
| 4th           | 295.23    | 0.0354 | 281.99        | 0.1544 | 280.70        | 0.1572 | 281.48        | 0.1690 |
| 5th           | 282.49    | 0.0422 | 270.77        | 0.0726 | 271.43        | 0.1043 | 271.54        | 0.0942 |
| 6th           | 268.00    | 0.1248 | 269.08        | 0.0828 | 269.39        | 0.0721 | 269.76        | 0.0827 |
| 7th           | 266.38    | 0.0547 | 265.83        | 0.1495 | 267.15        | 0.1325 | 267.09        | 0.1574 |
| 8th           | 263.04    | 0.2338 | 262.25        | 0.0272 | 262.33        | 0.0204 | 262.30        | 0.0237 |
| 9th           | 260.46    | 0.0052 | 257.98        | 0.1501 | 257.90        | 0.1417 | 258.24        | 0.1395 |
| 10th          | 256.83    | 0.0044 | 252.09        | 0.4278 | 252.00        | 0.4434 | 252.47        | 0.4665 |
| Ib            |           |       |               |       |               |       |               |       |
| 1st           | 380.67    | 0.0550 | 358.51        | 0.2333 | 359.53        | 0.2355 | 360.11        | 0.2472 |
| 2nd           | 359.65    | 0.1249 | 317.61        | 0.0335 | 322.09        | 0.0308 | 321.26        | 0.0332 |
| 3rd           | 303.14    | 0.0064 | 288.10        | 0.0108 | 289.45        | 0.0094 | 289.37        | 0.0110 |
| 4th           | 295.99    | 0.0326 | 282.96        | 0.2655 | 281.51        | 0.2756 | 282.34        | 0.2921 |
| 5th           | 284.14    | 0.0331 | 271.54        | 0.0726 | 272.35        | 0.1241 | 272.41        | 0.1144 |
| 6th           | 270.98    | 0.4253 | 269.78        | 0.0941 | 270.00        | 0.0689 | 270.41        | 0.0775 |
| 7th           | 267.85    | 0.0620 | 265.84        | 0.1524 | 267.88        | 0.1333 | 267.77        | 0.1608 |
| 8th           | 264.60    | 0.0683 | 263.74        | 0.0345 | 263.81        | 0.0125 | 263.74        | 0.0152 |
| 9th           | 262.39    | 0.0056 | 260.01        | 0.2014 | 259.90        | 0.1676 | 260.17        | 0.1667 |
| 10th          | 258.20    | 0.0078 | 254.20        | 0.4036 | 254.43        | 0.4355 | 254.93        | 0.4448 |
In both compounds, polarity of solvent affects wavelength and follows the same order, i.e. \( \lambda \) in DMSO > in water > in ethanol. Decrease in electronegativity increases the excited wavelengths in both phases because when electronegativity decreases the electron cloud slightly shifted toward HOMO and after that electron excited to LUMO by low energy.

**Frontier Molecular Orbital**

Highest occupied molecular orbital (HOMO) contains electrons and tends to donate these electrons such as an electron donor. On the other hand, lowest unoccupied molecular orbital (LUMO) contains free places and tends to accept electrons. The \( \lambda_{\text{max}} \) of compound formed due to excitation of electron from HOMO to LUMO. HOMO and LUMO in different phases for Ia and Ib shown in Figures 3 and 4, respectively.

![Figure 3: HOMO and LUMO of Ia (Isodensity value = 0.02).](image)

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In gas phase, HOMO was formed due to non-bonding (n) and pi-bonding electron density (switched on benzene ring containing hydroxyl group) but in solvent phase, HOMO was formed due to non-bonding (n) and pi-bonding electron density (switched on benzene ring containing halogen group). In both phases, LUMO was formed due to π* bonding electron density (switched on isoxazole ring and benzene ring) and electron transition was mixed type (n to π* and π to π*).

The molecular orbital energy gap was very important to study the photo-physics and kinetic stability of isoxazole compounds. E (LUMO), E (HOMO), and molecular orbital energy gap of Ia and Ib were shown in Table 3 in different phases.
Table 3: Energy gap (a.u.) for Ia and Ib.

| Solvent | E-LUMO | E-HOMO | Energy gap |
|---------|--------|--------|------------|
| Ia      |        |        |            |
| Gas phase | −0.093 | −0.240 | 0.147      |
| DMSO    | −0.083 | −0.238 | 0.155      |
| Ethanol | −0.083 | −0.238 | 0.155      |
| Water   | −0.082 | −0.237 | 0.155      |
| Ib      |        |        |            |
| Gas phase | −0.094 | −0.240 | 0.146      |
| DMSO    | −0.084 | −0.239 | 0.155      |
| Ethanol | −0.084 | −0.239 | 0.155      |
| Water   | −0.082 | −0.237 | 0.155      |

The molecular orbital energy gap decreased with a decrease in electronegativity of halogen group and the lowest molecular orbital energy gap (0.146 a.u.) was found in Ib gas phase. The molecular orbital energy gap was lower in gas phase than in solvent phase and no significance effect shown by solvent.

A large HOMO–LUMO gap implies high kinetic stability and low chemical reactivity because it is energetically unfavorable to add electrons to a high-lying LUMO. Meanwhile, a molecule with a small frontier orbital gap is more polarizable, is generally associated with a high chemical reactivity, low kinetic stability, and is termed as soft molecule [36].

Vibration Mode

The IR spectral data of Ia and Ib were recorded in Table 4. The calculated IR frequencies were show the difference with reported [37] value. The suggested reason is the computational data obtained when the Ia and Ib molecules in isolated state of vacuum condition and the reported values in solid phase. The phenolic O–H stretching frequency increased with decrease in electronegativity of halogen group, due to which more electronegative fluorine atom in Ia attracted the electron cloud on oxygen atom toward itself and phenolic O–H stretching was less from electron interaction.
Table 4: IR spectral data of Ia and Ib.

| Type              | Vibration mode | Frequency (cm\(^{-1}\)) | Ia       | Ib       | Reported |
|-------------------|---------------|--------------------------|----------|----------|----------|
| Isoxazole ring    | N–O str.      | 1,014.75                 | 1,015.32 | 850–800  |
|                   | C=N str.      | 1,555.15                 | 1,554.59 | 1,690–1,640 |
| Amine             | N–H Str.      | 3,589.04                 | 3,584.64 | 3,400–3,200 |
| Phenolic OH       | O–H Str.      | 3,319.27                 | 3,323.84 | 3,200–3,600 |
| Carbonyl          | C=O Str.      | 1,751.17                 | 1,752.53 | 1,650–1,800 |

**Thermo-Chemical Study**

The thermo-chemical parameters were calculated to their ideal gas state at 298.15 K and 101.325 kPa for Ia and Ib, respectively. The thermodynamic parameters including total electronic energy (\(E_t\)), enthalpy (\(H^{\Theta}\)), entropy (\(S^{\Theta}\)), Gibbs free energy (\(G^{\Theta}\)), and standard heat capacity at constant volume (\(C_{v}^{\Theta}\)) were obtained from the Gaussian frequency output files (Table 5). The equations used for computing thermo-chemical data in Gaussian programs have derived from statistical thermodynamics [38]. The thermal energy (\(E_{\text{thermal}}\)) calculated as the sum of zero-point energy and thermal energy corrections for molecular translation (\(E_{\text{trans}}\)), rotation (\(E_{\text{rot}}\)), and vibration (\(E_{\text{vib}}\)). The enthalpy (\(H^{\Theta}\)) was obtained by adding \(RT\) to the total electronic energy (\(E_t\)) and thermal energy at 298.15 K and 101.325 kPa.

Table 5: Thermo-dynamical properties of I (a, b).

| Properties          | Thermo-dynamical properties |
|---------------------|-----------------------------|
|                     | Ia                          | Ib                          |
| \(E_t\) (Hartree)   | -2,200.1584                 | -2,560.4430                 |
| \(H^{\Theta}\) (Hartree) | -2,199.3851             | -2,559.9730                 |
| \(G^{\Theta}\) (Hartree) | -2,199.4581                 | -2,559.7462                 |
| \(C_{v}^{\Theta}\) (cal/mole-K) | 83.292                  | 83.970                      |
| \(S^{\Theta}\) (cal/mole-K) | 153.511                    | 154.181                     |

With decrease in electronegativity of halogen group, the values of \(E_t\), \(H^{\Theta}\), and \(G^{\Theta}\) decreased and the value of \(C_{v}^{\Theta}\) and \(S^{\Theta}\) increased. It has known that the compounds with higher free energies are less stable than those with lower free energies. The Ib was more stable because it had low free energy i.e. -2559.7462 Hartree.
Conclusion

The DFT method reveals the useful information about the effect of solvent on electronic absorption spectra. There is less effect of electronegativity on structural, spectrophotometric, and thermo-chemical properties of fluorine- and chlorine-substituted isoxazoles. The chlorine (less electronegative)-substituted isoxazole (Ib) is soft molecule, more polarizable, high chemical reactivity, low kinetic stability, and high $\lambda_{\text{max}}$ than Ia.

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Table S1: Full geometry parameter of 1a.

| #  | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X     | Y     | Z     |
|----|--------|----|----|----|------|-------|----------|-------|-------|-------|
| 1  | C      | ----| ----| ----| -----| ------| ---------| -----  | -----  | -----  |
| 2  | C      | 1   | ----| ----| 1.382086 | ---- | ---------| 4.452798 | -1.431318 | 1.099516 |
| 3  | C      | 2   | 1   | 1.397135 | 120.056125 | ---- | 2.481565 | -0.621173 | -0.020434 |
| 4  | C      | 3   | 2   | 1.406247 | 120.426968 | 0.479239 | 3.276110 | 0.065870  | -0.955421 |
| 5  | C      | 4   | 3   | 1.402798 | 117.710470 | 1.567976 | -6.691666 | -0.049797 | -0.837694 |
| 6  | C      | 5   | 4   | 1.384907 | 121.975184 | 1.355191 | 5.260932  | -0.787056 | 0.174348  |
| 7  | H      | 2   | 1   | 6    | 1.082585 | 120.429447 | 177.816839 | 2.449900  | -1.895296 | 1.708520  |
| 8  | H      | 5   | 4   | 1.082753 | 120.033349 | 179.354848 | 6.339952  | -0.846577 | 0.241640  |
| 9  | H      | 6   | 5   | 1.336873 | 123.180462 | 178.622448 | 2.766799  | 0.768184  | -1.972567 |
| 10 | H      | 9   | 4   | 3    | 0.987299 | 108.011815 | 48.857739  | 2.060679  | 1.357294  | -1.613449 |
| 11 | Cl     | 5   | 4   | 3    | 1.729089 | 118.893274 | 178.834871 | 5.674839  | 0.757519  | -1.989480 |
| 12 | Cl     | 1   | 2   | 3    | 1.738641 | 119.795319 | 179.538607 | 5.185048  | -2.344943 | 2.384807  |
| 13 | C      | 3   | 2   | 1    | 1.478123 | 116.677663 | 173.434406 | 1.011704  | -0.717943 | -0.12873 |
| 14 | C      | 3   | 2   | 1    | 1.440120 | 132.186881 | 124.318323  | -0.026415 | 0.280181  | -0.144551 |
| 15 | C      | 4   | 3   | 1    | 1.395617 | 102.588657 | 175.002960  | -1.189415 | -0.490604 | -0.177251 |
| 16 | D      | 15  | 14  | 13   | 1.322159 | 109.895096 | 0.651558  | -0.877726  | -1.775498 | -0.178680 |
| 17 | N      | 13  | 3   | 2    | 1.304285 | 115.912624 | 26.072503  | 0.517894  | -1.925134 | -0.141547 |
| 18 | C      | 4   | 13  | 3    | 1.447956 | 129.069834 | 8.308636  | 0.094452  | 1.722547  | -0.183883 |
| 19 | D      | 18  | 14  | 13   | 1.230044 | 122.019273 | 26.696293  | 1.066479  | 2.282021  | -0.689017 |
| 20 | C      | 18  | 14  | 13   | 1.490902 | 119.644494 | 153.508025 | -0.986192  | 2.569242  | 0.397586  |
| 21 | C      | 20  | 18  | 14   | 1.397996 | 121.659248 | 40.184742  | -1.623498  | 2.226443  | 1.593714  |
| 22 | C      | 20  | 18  | 14   | 1.397474 | 118.546736 | 143.765401 | -1.303934  | 3.774113  | -0.235074 |
| 23 | C      | 21  | 20  | 18   | 1.389616 | 120.052229 | 176.629069 | -2.577370  | 3.075233  | 2.142090  |
| 24 | H      | 21  | 20  | 18   | 1.085866 | 119.727866 | 1.692445  | -1.350324  | 1.308557  | 2.105541  |
| 25 | C      | 22  | 20  | 18   | 1.387174 | 120.079220 | 177.891287 | -2.273602  | 4.607382  | 0.303124  |
| 26 | H      | 22  | 20  | 18   | 1.084646 | 118.861076 | 1.887969  | -0.778150  | -4.042161 | -1.145106 |
| 27 | C      | 23  | 21  | 20   | 1.391286 | 119.990201 | 0.755485  | -2.909543  | -4.259514 | 1.491847 |
| 28 | H      | 23  | 21  | 20   | 1.084828 | 119.856044 | 178.666561 | -3.054243  | 2.816546  | 3.081518  |
| 29 | H      | 25  | 22  | 20   | 1.084812 | 119.901812 | 179.197603 | -2.522725  | 5.535806  | -0.197398 |
| 30 | H      | 27  | 23  | 21   | 1.085176 | 119.874438 | 179.695245 | -3.658211  | 4.918938  | 1.918769  |
Table S2: Full geometry parameter of 1b.

| #  | Symbol | NA  | NB  | NC  | Bond          | Angle  | Dihedral     | X     | Y     | Z     |
|----|--------|-----|-----|-----|---------------|--------|--------------|-------|-------|-------|
| 1  | C      | 1   | 1   | 1   | 1.3841843     | 119.352851 | 197.984082 | -7.23676 | -2.908698 | -0.521712 |
| 2  | C      | 1   | 1   | 1   | 1.083787      | 120.572067 | 120.842924 | 0.560729 | -2.751786 | -0.49257 |
| 3  | C      | 1   | 1   | 1  | 1.0830940     | 119.724963 | 119.9719007 | -7.014539 | -0.340517 | -0.289115 |
| 4  | C      | 1   | 1   | 1  | 1.384891      | 121.974100 | 177.838636 | 2.609227 | -1.942041 | 1.737803 |
| 5  | C      | 1   | 1   | 1  | 1.082761      | 120.031942 | 179.373622 | 6.546574 | -1.199602 | 0.211342 |
| 6  | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 3.071472 | 0.620054 | -1.999691 |
| 7  | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 8  | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 9  | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 10 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 11 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 12 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 13 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 14 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 15 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 16 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 17 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 18 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |
| 19 | C      | 1   | 1   | 1  | 1.384913      | 121.974100 | 178.489272 | 0.731361 | 1.999691 | -1.999691 |

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|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 20 | C | 18 | 14 | 13 | 1.490525 | 119.603594 | -153.439324 | -0.511550 | 2.733800 | 0.377086 |
| 21 | C | 20 | 18 | 14 | 1.398021 | 121.616036 | 40.196388 | -1.153425 | 2.459721 | 1.588424 |
| 22 | C | 20 | 18 | 14 | 1.397492 | 118.603023 | -143.647799 | -0.754532 | 3.945201 | -0.275947 |
| 23 | C | 21 | 20 | 18 | 1.389620 | 120.061067 | 176.713205 | -2.037766 | 3.383461 | 2.132197 |
| 24 | H | 21 | 20 | 18 | 1.085903 | 119.760447 | -1.587452 | -0.937370 | 4.158265 | -1.198461 |
| 25 | C | 22 | 20 | 18 | 1.397492 | 118.603023 | -143.647799 | -0.754532 | 3.945201 | -0.275947 |
| 26 | H | 22 | 20 | 18 | 1.084672 | 118.873035 | 1.807575 | -0.225302 | 4.158265 | -1.198461 |
| 27 | C | 23 | 21 | 20 | 1.391245 | 119.959972 | 0.813531 | -2.297385 | 4.574651 | 1.461953 |
| 28 | H | 23 | 21 | 20 | 1.084811 | 119.849403 | -178.657381 | -2.517284 | 1.144335 | -0.201043 |
| 29 | H | 25 | 22 | 20 | 1.084819 | 119.883855 | -179.157027 | -1.853252 | 5.787263 | -0.258926 |
| 30 | H | 27 | 23 | 21 | 1.085158 | 119.883855 | 176.49728 | -2.992510 | 5.292669 | 1.884823 |
| 31 | N | 15 | 14 | 13 | 1.345225 | 130.917462 | -176.824851 | -2.207380 | 0.137847 | -0.201043 |
| 32 | H | 31 | 15 | 14 | 1.010466 | 113.743017 | -6.338537 | -2.283417 | 0.233487 | -0.193040 |
| 33 | C | 31 | 15 | 14 | 1.398479 | 116.269285 | 174.555158 | -4.585770 | 0.137847 | -0.201043 |
| 34 | C | 33 | 31 | 15 | 1.398479 | 116.269285 | 174.555158 | -4.585770 | 0.233487 | -0.193040 |
| 35 | C | 33 | 31 | 15 | 1.398479 | 116.269285 | 174.555158 | -4.585770 | 0.233487 | -0.193040 |
| 36 | C | 33 | 31 | 15 | 1.398479 | 116.269285 | 174.555158 | -4.585770 | 0.233487 | -0.193040 |
| 37 | H | 34 | 33 | 31 | 1.086516 | 119.831079 | -0.696026 | -4.502106 | 0.233487 | -0.193040 |
| 38 | C | 35 | 33 | 31 | 1.388917 | 119.745909 | -179.251658 | -4.812747 | 0.233487 | -0.193040 |
| 39 | H | 35 | 33 | 31 | 1.080016 | 120.938034 | 0.666372 | -2.670959 | 0.233487 | -0.193040 |
| 40 | C | 38 | 35 | 33 | 1.386400 | 120.417147 | 0.065467 | -5.950667 | 0.233487 | -0.193040 |
| 41 | H | 36 | 34 | 33 | 1.083460 | 120.373981 | -179.936271 | -6.731391 | 0.233487 | -0.193040 |
| 42 | H | 38 | 35 | 33 | 1.083615 | 119.660797 | 179.985300 | -4.905563 | 0.233487 | -0.193040 |
| 43 | Cl | 40 | 38 | 35 | 1.736180 | 119.944853 | -179.980915 | -7.521339 | 0.233487 | -0.193040 |