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# FT-Raman, FT-IR spectra and total energy distribution of 3-pentyl-2,6-diphenylpiperidin-4-one: DFT method

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#### ABSTRACT

FT-Raman and FT-IR spectra were recorded for 3-pentyl-2,6-diphenylpiperidin-4-one (PDPO) sample in solid state. The equilibrium geometries, harmonic vibrational frequencies, infrared and the Raman scattering intensities were computed using DFT/6-31G(d,p) level. Results obtained at this level of theory were used for a detailed interpretation of the infrared and Raman spectra, based on the total energy distribution (TED) of the normal modes. Molecular parameters such as bond lengths, bond angles and dihedral angles were calculated and compared with X-ray diffraction data. This comparison was good agreement. The intra-molecular charge transfer was calculated by means of natural bond orbital analysis (NBO). Hyperconjugative interaction energy was more during the  $\pi$ - $\pi$ \* transition. Energy gap of the molecule was found using HOMO and LUMO calculation, hence the less band gap, which seems to be more stable. Atomic charges of the carbon, nitrogen and oxygen were calculated using same level of calculation.

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#### 1. Introduction

Piperidones exhibit a wide spectrum of biological activities and form an essential part of the molecular structures of important drugs. Molecular geometry critically influences biological activity. Attention has been focused on structure-activity relationships. Piperidines with crowded groups at C<sub>3</sub> and C<sub>5</sub> have enhanced biological activity compared to other piperidines [1]. 2,6-Disubstituted piperidin-4-ones are regarded as an important framework and served as precursors for chiral biologically active natural alkaloids [2]. The biological activities of piperidones were found to be excellent if 2- and/or 6-positions are occupied by aryl groups [3]. Accordingly, anti-bacterial and anti-fungal activities of 2,6-diarylpiperidin-4-ones and their derivatives have been explored well [4,5]. Stereochemistry of N-benzoyl-2r,6c-diphenylpiperidin-4-one oxime, N-benzoyl-3t-methyl-2r,6c-diphenylpiperidin-4-one oxime, N-benzoyl-3tethyl-2r,6c-diphenylpiperidin-4-one oxime (3), N-acetyl-2r,6cdiphenylpiperidin-4-one oxime and N-acetyl-3t-methyl-2r,6cdiphenylpiperidin-4-one oxime have been studied using <sup>1</sup>H, <sup>13</sup>C and two-dimensional NMR spectra [6]. The main goal of this work is to record, simulate and interpret the vibrational spectra for the title compound, which has not been presented before. We also wanted to shed a light on the crystal and vibrational spectral data (FT-Raman and FT-IR) with the results of theoretical calculations.

#### 2. Experimental details

#### 2.1. Synthesis of 3-pentyl-2,6-diphenylpiperidin 4-one (PDPO) [7]

A mixture of ammonium acetate (3.85 g, 0.05 mol), benzaldehyde (10.6 ml, 0.1 mol) and 2-octanone (6.4 ml, 0.05 mol) in distilled ethanol was heated to boiling. After cooling the viscous liquid obtained was dissolved in diethyl ether (200 ml) and was shaken with 2 ml concentrated hydrochloric acid. The precipitated hydrochloride of the title compound was removed by filtration and washed with 40 ml mixture of ethanol and diethyl ether (1:1) and then with diethyl ether to remove most of the coloured impurities [7]. The base was liberated from an alcoholic solution by adding aqueous ammonia and then diluted with water. It was purified by column chromatography, using a n-hexane-ethyl acetate mixture as the solvent. The yield of the compound was 80%.

# 2.2. FT-Raman and FT-IR measurement

The FT-Raman spectrum of PDPO was recorded using the 1064 nm line of Nd:YAG laser as excitation wavelength in the region  $10-3500 \, \mathrm{cm}^{-1}$  on a Bruker model RFS100/S spectrophotometer

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**Fig. 1.** (a) Relative energy–dihedral angle curve in  $C_{36}-C_{39}$  bond. (b) Relative energy–dihedral angle curve in  $C_5-C_{35}$  bond. (c) Relative energy–dihedral angle curve in  $C_4-C_{13}$  bond. (d) Relative energy–dihedral angle curve in  $C_3-C_{24}$  bond. (e) Relative energy–dihedral angle curve in  $C_{39}-C_{42}$  bond. (f) Relative energy–dihedral angle curve in  $C_{42}-C_{47}$  bond.

equipped with FRA 106 FT-Raman module accessory. The spectral measurements were carried out at Sree Chitra Tirunal Institute for Medical Sciences and Technology, Poojappura, Thiruvananthapuram, Kerala, India. The FT-IR spectrum of this compound was recorded in the region 400–4000 cm<sup>-1</sup> on an IFS 66 V spectrophotometer using the KBr pellet technique. The spectrum was recorded at room temperature, with a scanning speed of 10 cm<sup>-1</sup> per minute and at the spectral resolution of 2.0 cm<sup>-1</sup> in CISL Laboratory, Annamalai University, Tamil Nadu, India.

# 3. Computational details

The entire calculations were performed at DFT levels on a Pentium 1 V/3.02 GHz personal computer using Gaussian 03W [8]

program package, invoking gradient geometry optimization [8,9]. Initial geometry generated from standard geometrical parameters was minimized without any constraint in the potential energy surface at DFT level, adopting the standard 6-31G(d,p) basis set. The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. Then, vibrationaly averaged nuclear positions of PDPO were used for harmonic vibrational frequency calculations resulting in IR and Raman frequencies together with intensities and Raman depolarization ratios. In this study, the DFT method (B3LYP) was used for the computation of molecular structure, vibrational frequencies and energies of optimized structures. The vibrational modes were assigned on the basis of TED analysis using som program [10].



Fig. 2. Optimized molecular structure of 3-pentyl-2, 6-diphenylpiperidin-4-one.

It should be noted that Gaussian 03W package able to calculate the Raman activity. The Raman activities were transformed into Raman intensities using Raint program [11] by the expression:

$$I_i = 10^{-12} \frac{(\nu_0 - \nu_i)^4}{\nu_i \cdot S} \tag{1}$$

where  $I_i$  is the Raman intensity, *S* is the Raman scattering activities,  $v_i$  is the wavenumber of the normal modes and  $v_0$  denotes the wavenumber of the excitation laser [12].

# 4. Results and discussion

#### 4.1. Conformational analysis

The chair conformer of piperidine molecule is the most stable conformer. Therefore, we neglected other conformations that differ from the chair (boat, envelope or twist boat) because of their high energy. Moreover, it has two possible chair conformations, which differ in the axial (A) or equatorial (E) positions of the N-H group [13–15]. Piperidine molecules show the equatorial form of NH of chair conformer as the most stable. Piperidine molecule adopts the NH equatorial position of the chair conformer. Then, in order to reveal all possible conformations of studied molecule, a detailed potential energy surface (PES) scan in six dihedral angles was performed. This scan was carried out by relaxed PES scanning calculations in all geometrical parameters by changing the torsion angle for every  $10^{\circ}$  rotation around the bond. The shape of the potential energy as a function of the dihedral angle is illustrated in Fig. 1a–f. The curves between relative energy and dihedral angles  $(a \rightarrow H_{11}-C_3-C_{24}-C_{25} \text{ and } c \rightarrow H_9-C_4-C_{13}-C_{14})$  are shown in Fig. 1a and c. As seen in Fig. 1a and c,  $H_{11}$ - $C_3$ - $C_{24}$ - $C_{25}$  dihedral angle of phenyl ring is attached with  $C_3$  is determined at  $160^\circ$  for B3LYP level of theory. H<sub>9</sub>-C<sub>4</sub>-C<sub>13</sub>-C<sub>14</sub> dihedral angle is predicted at 10°. In the optimized structure, H<sub>11</sub>-C<sub>3</sub>-C<sub>24</sub>-C<sub>25</sub> and H<sub>9</sub>-C<sub>4</sub>-C<sub>13</sub>-C<sub>14</sub> dihedral angles are predicted at 162.24° and 9.50°, respectively.

#### 4.2. Molecular geometry

The optimized geometrical parameters and structure of PDPO was calculated at 6-31G(d,p) level, are given in Table 1 and Fig. 2, respectively. Geometrical parameters such as bond lengths, bond angles and dihedral angles are also given along with its single crystal X-ray diffraction data. The bond length of  $C_1$ – $O_{50}$  is about 1.218 in B3LYP method. And its corresponding experimental value



Fig. 3. Theoretical (a) and experimental (b) FT-IR spectrum of PDPO.

is 1.214Å [7]. Similarly the C<sub>3</sub>-N<sub>12</sub> and C<sub>4</sub>-N<sub>12</sub> bond distances are calculated at 1.465 and 1.470 Å (DFT), which are in agreement with X-ray data. The bond distance of C-C is usually observed as ~1.400 Å. In the present investigation, bond lengths of  $C_1$ – $C_2$ ,  $C_1-C_5$ ,  $C_2-C_3$ ,  $C_3-C_{24}$ ,  $C_4-C_5$ ,  $C_4-C_{13}$  and  $C_5-C_{35}$  are in line with literature values. On the other hand, the bond distances ( $C_{13}$ – $C_{14}$ ,  $C_{13}-C_{15}, C_{14}-C_{16}, C_{15}-C_{18}, C_{16}-C_{20}, C_{18}-C_{20}, C_{25}-C_{27}, C_{26}-C_{29}, C_{18}-C_{18} C_{27}-C_{31}$  and  $C_{29}-C_{31}$ ) of the sixmembered rings are approximately 1.39 Å/B3LYP with few exceptions. These values are in agreement with literature values [7]. Crystal data [7] reveal that the C-H bond distances are  $\sim$ 1.00 Å, which is supported by the calculated values. The calculated angles 121.85° and 122.91° (DFT), are belongs to  $C_2-C_1-O_{50}$  and  $C_5-C_1-O_{50}$ , respectively. And their corresponding literature values are 121.93° and 122.01°. These larger bond angles are may be due to electron density in oxygen atom. The bond angle  $C_{14}$ - $C_{13}$ - $C_{15}$ : 118.705/B3LYP is less when comparing with other bond angles  $C_{13}-C_{14}-C_{16}$ ,  $C_{13}-C_{15}-C_{18}$ ,  $C_{14}-C_{16}-C_{20}$ ,  $C_{15}-C_{18}-C_{20}$  and  $C_{16}-C_{20}-C_{18}$  (~120°). It may be due to the phenyl ring is attached with C<sub>4</sub>. Similar trend has been observed in the second phenyl ring. The bond angles of C–C–H are  ${\sim}109^{\circ}$  except in both phenyl rings ( $\sim 120^{\circ}$ ) which are in agreement with literature values [7]. The dihedral angles of title molecule were calculated, and some of them were compared with available X-ray diffraction data as shown in Table 1.

# 4.3. Vibrational assignments

Synthesized PDPO, consists 51 atoms and hence 147 normal modes of vibrations and the molecule belongs to  $C_1$  symmetry. The fundamental vibrational wavenumbers of PDPO was calculated by DFT (B3LYP/6-31G(d,p)) is given in Table 2. The resulting vibrational wavenumbers for the optimized geometries, IR intensities as well as Raman scattering activities and experimental FT-IR, FT-Raman frequencies are also listed. Experimental and theoretical spectra of title compound have been shown in Fig. 3 (FT-IR) and Fig. 4 (FT-Raman). The normal modes of vibration were assigned on the basis of TED. To bring the theoretical values closer to experimental values, we used the scale factor: 0.9608.

#### 4.3.1. N–H vibrations

The N–H stretching vibration [13,14] appears strongly and broadly in the region 3500–3300 cm<sup>-1</sup>.Y. Erdogdu et al., assigned  $\nu_{\rm N–H}$  mode in the region 3500–3300 cm<sup>-1</sup> [15]. In this study, the frequency was observed as weak and narrow band in both FT-IR and FT-Raman, where the frequencies are attributed to 3316 cm<sup>-1</sup> and

# Table 1

Bond lengths, bond angles and dihedral angles of PDPO.

$ \begin{array}{ccccccc} c_1 c_2 & - L24 & - L218 & - C_1 C_2 & - L22 & -$	Parameters Bond length (Å)	Exp.ª	B3LYP/6-31G(d,p)	Parameters Angles Contd.	Exp. <sup>a</sup>	B3LYP/6-31G(d,p)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_1 = O_{E0}$	1 214	1 218	$C_{E} - C_{1} - O_{E0}$	122.0	122.9
$\begin{array}{c} c_{-}c_{1}\\ c_{-}c_{2}\\ c_{-}c_{3}\\ c_{-}c_{4}\\ c_{-}c_{5}\\ c_{-}c_{-}c_{5}\\ c_{-}c_{-}c_{-}c_{-}c_{-}c_{-}c_{-}c_{-}$	$C_{2} = N_{12}$	1.211	1 465	$C_1 = C_2 = H_2$	109.0	109.3
$\begin{array}{cccccc} c_1 c_2 c_2 c_3 c_4 c_4 c_4 c_4 c_4 c_4 c_4 c_4 c_4 c_4$	C4-N12	1.105	1 470	$C_1 - C_2 - H_7$	109.0	109.1
$\begin{array}{ccccccc} C_1 C_2 C_2 C_1 C_2 C_2 C_1 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2$	$C_4 = C_1$	1.506	1,470	$C_1 - C_2 - H_c$	109.0	108.1
$\begin{array}{cccccc} c_1 & 1.572 & 1.548 & r_1, c_2, r_1, & 100.0 & 1000 \\ C_{-C_0} & 1.570 & 1.577 & C_1-C_{+}r_1 & 100.0 & 1073 \\ C_{-C_0} & 1.510 & 1.578 & C_1-C_{+}r_1 & 100.0 & 1073 \\ C_{-C_0} & 1.530 & 1.547 & R_1-C_1-R_1 & 100.0 & 1073 \\ C_{-C_0} & 1.330 & 1.400 & R_1-C_1-R_1 & 100.0 & 1073 \\ C_{-C_0} & 1.330 & 1.400 & R_1-C_1-R_1 & 100.0 & 1073 \\ C_{-C_0} & 1.331 & 1.402 & C_1-C_1+r_1 & 100.0 & 1068 \\ C_{-C_0} & 1.337 & 1.366 & C_1-C_1+r_0 & 100.0 & 1073 \\ C_{-C_0} & 1.331 & 1.347 & R_1-C_1-R_1 & 100.0 & 10683 \\ C_{-C_0} & 1.337 & 1.366 & C_{-C_1}-R_1 & 100.0 & 1088 \\ C_{-C_0} & 1.331 & 1.385 & R_1-C_1-R_1 & 100.0 & 1085 \\ C_{-C_0} & 1.331 & 1.385 & C_1-C_1+r_1 & 100.0 & 1085 \\ C_{-C_0} & 1.332 & 1.385 & C_1-C_1+r_1 & 100.0 & 1085 \\ C_{-C_0} & 1.522 & 1.335 & C_1-R_1-r_1 & 100.0 & 1085 \\ C_{-C_0} & 1.522 & 1.533 & C_1-R_1-r_1 & 100.0 & 1085 \\ C_{-C_0} & 1.522 & 1.533 & C_1-R_1-r_1 & 100.0 & 1083 \\ C_{-C_0} & 1.522 & 1.533 & C_1-R_1-r_1 & 100.0 & 100.0 \\ C_{-C_0} & 1.522 & 1.533 & C_1-R_1-r_1 & 100.0 & 100.0 \\ C_{-C_0} & 1.522 & 1.533 & C_1-R_1-r_1 & 120.0 & 110.0 \\ C_{-C_0} & 1.521 & 1.514 & C_{1-C_0}-r_1, & 120.0 & 110.0 \\ C_{-C_0} & 1.521 & 1.514 & C_{1-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.520 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.520 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.50 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.50 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{0-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.007 & C_{-C_0}-r_1, & 120.0 & 100.0 \\ C_{-C_0} & 1.00 & 1.00$	$C_1 - C_2$	1 526	1 531	$C_{2} - C_{2} - H_{7}$	109.0	111.1
$\begin{array}{ccccccc} C_1 C_2 C_1 C_1 C_1 C_1 C_2 C_1 C_1 C_1 C_2 C_2 C_1 C_1 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2$	$C_1 = C_2$	1.520	1 549	$H_{c} - C_{2} - H_{7}$	109.0	109.0
$\begin{array}{ccccccc} c_1 & 1550 & 1567 & C_1 C_2 C_2 N_0 & 1074 & 1073 \\ C_1 C_1 & 1511 & 1519 & H_1 C_1 C_3 & 1080 & 1135 \\ C_1 C_4 & 1390 & 1400 & N_2 C_1 C_4 & 1080 & 1135 \\ C_1 C_4 & 1390 & 1400 & N_2 C_4 C_4 & 1080 & 1088 \\ C_1 C_4 & 1392 & 1393 & 1486 & C_1 C_4 N_1 & 1080 & 1088 \\ C_2 C_4 & 1392 & 1394 & H_2 C_4 C_4 & 1080 & 1077 \\ C_2 C_6 & 1392 & 1394 & H_2 C_4 C_4 & 1080 & 1077 \\ C_2 C_6 & 1392 & 1394 & H_2 C_4 C_4 & 1080 & 1077 \\ C_2 C_6 & 1392 & 1394 & H_2 C_4 C_5 & 1080 & 1077 \\ C_2 C_6 & 1392 & 1394 & H_2 C_4 C_5 & 1080 & 1077 \\ C_2 C_6 & 1392 & 1394 & H_2 C_4 C_5 & 1080 & 1077 \\ C_2 C_6 & 1393 & 1385 & C_1 C_4 C_7 & 1080 & 1063 \\ C_2 C_6 & 1392 & 1395 & C_1 C_4 C_7 & 1010 & 1066 \\ C_2 C_6 & 1522 & 1533 & C_1 N_4 C_4 & 1110 & 1095 \\ C_6 C_6 & 1522 & 1533 & C_1 N_4 C_4 & 1110 & 1095 \\ C_6 C_6 & 1522 & 1533 & C_1 N_4 C_4 & 1110 & 1095 \\ C_6 C_6 & 1526 & 1533 & C_1 C_4 C_6 H_1 & 1020 & 1139 \\ C_6 C_6 & 1526 & 1533 & C_1 C_4 C_6 H_1 & 1200 & 1139 \\ C_6 C_6 & 1526 & 1533 & C_1 C_4 C_6 H_1 & 1200 & 1139 \\ C_6 C_6 & 1526 & 1077 & C_6 C_6 H_2 & 1200 & 1139 \\ C_6 C_6 & 1528 & 1007 & C_6 C_6 H_2 & 1200 & 1139 \\ C_6 C_6 & 1538 & 1088 & C_6 C_6 H_2 & 1200 & 1139 \\ C_6 C_1 & 1000 & 1107 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 1000 & 1107 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 1000 & 1007 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 1000 & 1088 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_2 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_2 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_2 & 1200 & 1137 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1200 & 1139 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1000 & 1083 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & 1000 & 1083 \\ C_6 H_1 & 0390 & 1088 & C_6 C_6 H_1 & $	$C_2 = C_3$	1.552	1 518	$C_2 = C_2 = H_{11}$	109.0	106.9
$\begin{array}{c} c_{-}c_{0} & 1.513 & 1.519 & H_{1}-c_{-}N_{0} & 1080 & 111.5 \\ c_{-}c_{1} & 1.513 & 1.519 & H_{1}-c_{-}N_{0} & 1080 & 111.5 \\ c_{-}c_{1} & 1.390 & 1.400 & N_{1}-c_{-}c_{2} & 111.2 & 110.9 \\ c_{-}c_{0} & 1.390 & 1.400 & N_{1}-c_{-}c_{2} & 111.2 & 110.9 \\ c_{-}c_{0} & 1.390 & 1.400 & N_{1}-c_{-}c_{1} & 110.0 & 106.6 \\ c_{-}c_{0} & 1.392 & 1.390 & c_{-}c_{-}A_{-}N_{0} & 100.1 & 108.1 \\ c_{-}c_{0} & 1.392 & 1.391 & N_{1}-c_{-}c_{-}C_{1} & 100.1 & 108.1 \\ c_{-}c_{-}c_{0} & 1.391 & 1.396 & c_{-}c_{-}A_{-}N_{0} & 100.2 & 109.1 \\ c_{-}c_{-}c_{-} & 1.393 & 1.395 & N_{1}-c_{-}C_{+} & 107.0 & 106.5 \\ c_{-}c_{-}c_{-} & 1.393 & 1.395 & c_{-}c_{-}A_{-}H_{0} & 107.0 & 105.5 \\ c_{-}c_{-}c_{-} & 1.393 & 1.395 & c_{-}A_{-}A_{-}H_{0} & 107.0 & 105.5 \\ c_{-}c_{-}c_{-} & 1.392 & 1.395 & c_{-}A_{-}H_{0} & 107.0 & 105.5 \\ c_{-}c_{-}c_{-} & 1.392 & 1.395 & c_{-}A_{-}H_{0} & 108.0 & 109.3 \\ c_{-}c_{-}c_{-} & 1.522 & 1.533 & c_{-}A_{-}H_{0} & 108.0 & 109.3 \\ c_{-}c_{-}c_{-} & 1.521 & 1.534 & c_{1}-c_{-}H_{0} & 108.0 & 109.1 \\ c_{-}c_{-}c_{-} & 1.522 & 1.552 & c_{-}c_{-}c_{-}H_{0} & 120.0 & 119.1 \\ c_{-}c_{-}c_{-} & 1.521 & 1.544 & c_{1}-c_{-}H_{0} & 120.0 & 119.1 \\ c_{-}c_{-}c_{-} & 1.522 & 1.552 & c_{-}c_{-}c_{-}H_{0} & 120.0 & 119.1 \\ c_{-}c_{-}h_{1} & 0.900 & 1.077 & c_{1}-c_{-}H_{0} & 120.0 & 109.1 \\ c_{-}c_{+}h_{1} & 0.900 & 1.077 & c_{1}-c_{-}H_{0} & 120.0 & 109.1 \\ c_{-}H_{0} & 0.901 & 1.077 & c_{1}-c_{-}H_{0} & 120.0 & 109.1 \\ c_{-}H_{0} & 0.901 & 1.086 & c_{1}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.901 & 1.086 & c_{-}c_{-}-H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.901 & 1.087 & c_{1}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.901 & 1.087 & c_{1}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.950 & 1.088 & c_{-}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.950 & 1.088 & c_{-}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.950 & 1.088 & c_{-}-c_{-}H_{0} & 120.0 & 120.1 \\ c_{-}H_{0} & 0.950 & 1.088 & c_{-}-c_{-}H_{0} & 100.0 & 103.1 \\ c_{-}H_{0} & 0.950 & 1.088 & c_{-}-c_{-}H_{0} & 100.0 & 103.1 \\ c_{-}H_{0} & 0.990 & 1.097 & c$	$C_{3} = C_{24}$	1.514	1.510	$C_2 = C_3 = N_{12}$	107.4	107.8
$\begin{array}{c} c_{n}c_{n}\\ c_{n}c_{n}\\$	$C_4 - C_5$	1.513	1.507	$C_2 = C_3 = N_{12}$	107.4	111.5
$ \begin{array}{c} c_1 - c_1 \\ c_1 - c_1 $	$C_4 - C_{13}$	1.515	1.515	$H_{11} = C_3 = R_{12}$	109.0	107.8
$\begin{array}{cccccc} 1 & 1387 & 1402 & C_1 C_4 + h_1 & 108 & 1066 \\ C_1 - C_6 & 1387 & 1366 & C_1 - C_4 h_2 & 100. & 111.5 \\ C_5 - C_6 & 1392 & 1394 & H_9 - C_4 + h_1 & 109. & 107.7 \\ C_6 - C_6 & 1392 & 1395 & H_9 - C_4 - C_1 & 108.7 & 108.1 \\ C_6 - C_6 & 1392 & 1395 & H_9 - C_4 - C_1 & 108.7 & 108.1 \\ C_6 - C_6 & 1391 & 1385 & C_1 - C_4 + h_6 & 107.7 & 108.4 \\ C_6 - C_7 & 1391 & 1385 & C_1 - C_4 + h_6 & 107.7 & 108.4 \\ C_6 - C_6 & 1292 & 1395 & H_9 - C_4 - C_1 & 10.7 & 108.4 \\ C_6 - C_6 & 1292 & 1395 & C_1 - H_6 & 107.7 & 108.4 \\ C_6 - C_6 & 1522 & 1515 & C_1 + h_9 - C_4 - C_1 & 10.7 & 1143 \\ C_8 - C_6 & 1522 & 1515 & C_1 + h_9 - 100 & 1199 \\ C_8 - C_6 & 1522 & 1515 & C_1 + h_9 - 100 & 1199 \\ C_8 - C_6 & 1522 & 1515 & C_1 + h_9 - 1200 & 1191 \\ C_8 - C_6 & 1522 & 1517 & C_1 - C_1 + h_9 & 1200 & 1191 \\ C_8 - C_6 & 1522 & 1517 & C_1 - C_1 + h_9 & 1200 & 1191 \\ C_8 - C_6 & 1590 & 1087 & C_1 - C_1 + h_9 & 1200 & 1191 \\ C_8 - H_9 & 009 & 1087 & C_1 - C_1 + h_9 & 1200 & 1191 \\ C_8 - H_9 & 1000 & 1.107 & C_1 - C_1 + H_9 & 1200 & 1193 \\ C_8 - H_9 & 1000 & 1.107 & C_1 - C_1 + H_9 & 1200 & 1193 \\ C_8 - H_9 & 1000 & 1.107 & C_1 - C_1 + H_9 & 1200 & 1193 \\ C_8 - H_9 & 009 & 1085 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 009 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1200 & 1193 \\ C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1000 & 1083 \\ C_8 - C_8 - H_9 & 0050 & 1085 & C_1 - C_8 - H_9 & 1000 & 1083 \\ C_8 - C_8 - H_9 & 0050 & 1086 & C_1 - C_8 - H_9 & 1000 & 1083 \\ C_8 - C_8 - $	C	1 300	1,00	$N_{11} = C_2 = C_{24}$	111.2	110.0
$\begin{array}{c} c_1 c_2 \\ c_1 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_2 c_2 \\ c_1 c_2 \\ c_1 c_1 \\$	$C_{13} = C_{14}$	1 303	1.400	$C_{12} = C_{12} = H_{12}$	109.0	106.6
$\begin{array}{ccccccc} 1 & 1302 & 1.384 & 1.4 $	C C	1.333	1,402	$c_5 - c_4 - H_9$	109.0	108.8
$\begin{array}{c} c_1 = C_0 & 1.392 & 1.385 & H_1 = C_1 C_1 & 100 & 107 \\ C_1 = C_0 & 1.378 & 1.397 & N_1 < C_1 & 108.7 & 106.1 \\ C_2 = C_0 & 1.391 & 1.395 & C_1 < C_2 + H_0 & 107.0 & 106.5 \\ C_3 = C_0 & 1.395 & 1.395 & C_1 < C_2 + H_0 & 107.0 & 106.5 \\ C_3 = C_0 & 1.372 & 1.385 & C_1 < C_2 + H_0 & 107.0 & 106.5 \\ C_3 = C_0 & 1.372 & 1.385 & C_1 + H_1 & 108 & 109.2 \\ C_3 = C_0 & 1.372 & 1.385 & C_1 + H_1 & 108 & 109.2 \\ C_3 = C_0 & 1.321 & 1.334 & C_1 - C_1 + H_1 & 108 & 109.2 \\ C_3 = C_0 & 1.321 & 1.334 & C_1 - C_1 + H_1 & 100 & 119.4 \\ C_3 = C_0 & 1.321 & 1.334 & C_1 - C_1 + H_1 & 1200 & 119.4 \\ C_3 = C_0 & 1.322 & 1.312 & C_1 - C_1 + H_2 & 1200 & 119.4 \\ C_4 = C_7 & 1.522 & 1.512 & C_1 - C_4 + H_1 & 1200 & 119.7 \\ C_4 = C_7 & 1.522 & 1.512 & C_1 - C_4 + H_1 & 1200 & 120.3 \\ C_4 = H_1 & 1.000 & 1.107 & C_4 - C_6 + H_2 & 120.0 & 120.3 \\ C_4 = H_1 & 1.000 & 1.107 & C_6 - C_6 + H_2 & 120.0 & 120.1 \\ H_2 + H_2 & 0.050 & 1.087 & C_4 - C_9 + H_2 & 120.0 & 120.1 \\ C_4 = H_1 & 0.000 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 120.1 \\ C_4 = H_4 & 0.050 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 120.1 \\ C_6 = H_1 & 0.050 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 120.1 \\ C_6 = H_2 & 0.550 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.086 & C_4 - C_9 + H_2 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.085 & C_6 - C_9 + H_2 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.085 & C_6 - C_9 + H_9 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.085 & C_6 - C_9 + H_9 & 120.0 & 119.7 \\ C_6 = H_6 & 0.550 & 1.085 & C_6 - C_9 + H_9 & 120.0 & 119.7 \\ C_6 = H_6 & 0.590 & 1.085 & C_6 - C_6 + H_9 & 120.0 & 119.7 \\ C_6 = H_6 & 0.590 & 1.085 & C_6 - C_6 + H_9 & 100.0 & 108.4 \\ C_6 = H_6 & 0.590 & 1.085 & C_6 - C_6 + H_9 & 100.0 & 108.4 \\ C_6 = H_6 & 0.590 & 1.086 & C_7 - C_9 + H_9 & 109.0 & 108.4 \\ C_6 = H_6 & 0.590 & 1.086 & C_7 - C_9 + H_9 & 109.0 & 108.4 \\ C_6 = H_6 & 0.590 & 1.086 & C_7 - C_9 + H_9 & 109.0 & 108.4 \\ C_6 = H_6 & 0.590 & 1.086 & C_7 - C_9 + H_9 & 109.0 & 108.4 \\ C_7 = C_6 - C_6 & 113.4 & 110$	$C_{14} - C_{16}$	1.307	1,390	$C_5 - C_4 - N_{12}$	109.5	108.8
$ \begin{array}{cccccc} 1 & 1378 & 1377 & 147 & 147 & 167 & 1067 & 1061 \\ C_{3}-C_{3} & C_{3}-C_{3} & 1336 & C_{1}-C_{1}-H_{10} & 1070 & 1053 \\ C_{3}-C_{3} & 1335 & 1335 & C_{1}-C_{1}-H_{10} & 1070 & 1053 \\ C_{3}-C_{3} & 1335 & 1335 & C_{1}-K_{1}-H_{1} & 1100 & 1093 \\ C_{3}-C_{1} & 1378 & 1336 & C_{1}-K_{1}-H_{1} & 1100 & 1093 \\ C_{3}-C_{4} & 1522 & 1333 & C_{1}-K_{1}-H_{1} & 1100 & 1093 \\ C_{3}-C_{4} & 1522 & 1333 & C_{1}-K_{1}-H_{1} & 1100 & 1093 \\ C_{3}-C_{4} & 1522 & 1333 & C_{1}-K_{1}-H_{1} & 1000 & 1107 \\ C_{3}-C_{4} & 0.990 & 1.097 & C_{1}-C_{1}-H_{1} & 1200 & 1180 \\ C_{3}-H_{4} & 0.990 & 1.097 & C_{1}-C_{1}-H_{2} & 1200 & 1203 \\ C_{3}-H_{4} & 0.990 & 1.097 & C_{1}-C_{4}-H_{1} & 1200 & 1203 \\ C_{3}-H_{4} & 0.990 & 1.097 & C_{4}-C_{4}-H_{2} & 1200 & 1203 \\ C_{3}-H_{4} & 0.990 & 1.007 & C_{3}-C_{1}-H_{2} & 1200 & 1203 \\ C_{3}-H_{4} & 0.990 & 1.007 & C_{3}-C_{1}-H_{2} & 1200 & 1203 \\ C_{3}-H_{4} & 0.990 & 1.007 & C_{3}-C_{1}-H_{2} & 1200 & 1201 \\ C_{4}-H_{5} & 0.910 & 1.107 & C_{5}-C_{1}-H_{2} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1187 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1187 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1187 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1200 & 1201 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1000 & 1032 \\ C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1000 & 1031 \\ C_{4}-C_{4}-H_{5} & 0.950 & 1.086 & C_{4}-C_{5}-H_{5} & 1000 & 1001 \\ C_{5}-H_{5} & 0.00 & 1003 & 00.0101 \\ C_{5}-H_{5} & 0.00 & 00.0103 \\$		1,352	1,354	$H_2 = C_4 - N_{12}$	109.0	107.7
$ \begin{array}{c} c_1 - c_2 - c_1 & 1.39 & 1.396 & c_1 - c_2 - h_1 & 1070 & 1063 \\ c_2 - c_2 & 1.395 & 1.395 & c_1 - c_2 - h_1 & 1070 & 1055 \\ c_2 - c_1 & 1.385 & 1.395 & c_1 - c_2 - h_1 & 1070 & 1085 \\ c_3 - c_1 & 1.379 & 1.386 & c_1 - h_2 - c_2 & 1117 & 1143 \\ c_5 - c_6 & 1.526 & 1.533 & c_1 - h_2 - h_4 & 1088 & 1092 \\ c_4 - c_6 & 1.526 & 1.533 & c_1 - h_2 - h_4 & 1088 & 1092 \\ c_4 - c_6 & 1.520 & 1.333 & c_1 - c_1 - h_1 & 1200 & 1157 \\ c_4 - h_1 & 0.00 & 1.007 & c_4 - c_4 - h_1 & 1200 & 1137 \\ c_4 - h_1 & 0.00 & 1.007 & c_4 - c_4 - h_1 & 1200 & 1137 \\ c_4 - h_1 & 0.00 & 1.107 & c_4 - c_4 - h_1 & 1200 & 1137 \\ c_4 - h_4 & 1.000 & 1.107 & c_4 - c_4 - h_1 & 1200 & 1203 \\ c_4 - h_4 & 1.000 & 1.107 & c_4 - c_4 - h_2 & 1200 & 1201 \\ c_4 - h_4 & 0.000 & 1.007 & c_4 - c_4 - h_2 & 1200 & 1201 \\ c_4 - h_4 & 0.000 & 1.007 & c_4 - c_4 - h_2 & 1200 & 1202 \\ c_5 - h_1 & 0.050 & 1.088 & c_1 - c_5 - h_2 & 1200 & 1202 \\ c_5 - h_1 & 0.050 & 1.088 & c_1 - c_5 - h_2 & 1200 & 1204 \\ c_4 - h_4 & 0.050 & 1.086 & c_1 - c_5 - h_2 & 1200 & 1204 \\ c_4 - h_4 & 0.500 & 1.086 & c_1 - c_5 - h_2 & 1200 & 1204 \\ c_5 - h_6 & 0.500 & 1.088 & c_7 - c_5 - h_2 & 1200 & 1204 \\ c_6 - h_2 & 0.500 & 1.086 & c_1 - c_5 - h_2 & 1200 & 1184 \\ c_6 - h_2 & 0.500 & 1.086 & c_1 - c_5 - h_2 & 1200 & 1184 \\ c_6 - h_2 & 0.500 & 1.086 & c_1 - c_5 - h_2 & 1200 & 1204 \\ c_6 - c_5 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1200 & 1185 \\ c_6 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1200 & 1204 \\ c_6 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1200 & 1201 \\ c_6 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1200 & 1201 \\ c_6 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1200 & 1201 \\ c_6 - h_8 & 0.500 & 1.086 & c_7 - c_5 - h_3 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000 & 1083 \\ c_6 - h_8 & 0.500 & 1.086 & c_6 - c_5 - h_4 & 1000$	$C_{16} - C_{20}$	1.332	1,395	$N_{12} = C_1 = C_{13}$	109.0	107.7
$ \begin{array}{c} c_{\alpha} - C_{\alpha} & 1.36 & 1.365 & c_{\alpha} - C_{\alpha} + B_{\alpha} & 1070 & 1053 \\ c_{\alpha} - C_{\alpha} & 1.379 & 1.386 & 1.385 & H_{\alpha} - C_{5} & 1080 & 1089 \\ c_{\alpha} - C_{\alpha} & 1.522 & 1.335 & C_{\alpha} - N_{\alpha} - H_{\alpha} & 1100 & 1005 \\ c_{\alpha} - C_{\alpha} & 1.521 & 1.334 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1100 & 1187 \\ c_{\alpha} - C_{\alpha} & 1.521 & 1.334 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1184 \\ c_{\alpha} - C_{\alpha} & 1.521 & 1.334 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - C_{\alpha} & 1.521 & 1.334 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - C_{\alpha} & 1.521 & 1.334 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - C_{\alpha} & 1.522 & 1.332 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - C_{\alpha} & 1.000 & 1.007 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.002 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.007 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.008 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.991 & 1.017 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1202 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1202 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - C_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1187 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1200 & 1202 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1000 & 1087 \\ c_{\alpha} - H_{\alpha} & 0.950 & 1.086 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108.5 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.097 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108.5 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.096 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108.5 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.096 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108.5 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.096 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108.5 \\ c_{\alpha} - H_{\alpha} & 0.990 & 1.096 & C_{\alpha} - C_{\alpha} - H_{\alpha} & 1080 & 108$	$C_{18} = C_{20}$	1.378	1,397	$N_{12} - C_4 - C_{13}$	108.7	105.1
$ \begin{array}{c} c_{\alpha} - C_{\alpha} & c_{\alpha} + c_{\alpha} + c_{\alpha} + c_{\alpha} & c_{\alpha} & c_{\alpha} + c_{\alpha} $	$C_{25} - C_{27}$	1,391	1,390	$C_1 - C_5 - \Pi_{10}$	107.0	105.5
$\begin{array}{ccccccc} C_{2} C_{2} C_{2} C_{3} C_{4} C_{5} C_{5}$	$C_{26} - C_{29}$	1.595	1,595	$C_4 - C_5 - \Pi_{10}$	107.0	105.5
$ \begin{array}{c} C_{\alpha} - C_{\alpha} & (1,3) + (1,3) $	$C_{27} - C_{31}$	1.365	1,393	$\Pi_{10} - C_5 - C_{35}$	109.0	114.2
$\begin{array}{c} Lis-Lis & 1.322 & 1.333 & Lis-N_2-His & 10.0 & 10.95 \\ Car \cdot Car & 1.525 & 1.533 & Car \cdot Car +His & 10.88 & 10.24 \\ Car \cdot Car & 1.522 & 1.533 & Car \cdot Car +His & 10.0 & 11.97 \\ Car \cdot Car & 1.999 & 10.997 & Car \cdot Car +His & 120.0 & 120.3 \\ Car \cdot Car & 1.999 & 10.997 & Car \cdot Car +His & 120.0 & 120.3 \\ Car \cdot Lar & 0.999 & 10.997 & Car \cdot Car +His & 120.0 & 120.3 \\ Car \cdot Lar & 0.000 & 1.107 & Car \cdot Car +His & 120.0 & 120.3 \\ Car \cdot His & 1.000 & 1.107 & Car \cdot Car +His & 120.0 & 120.3 \\ Car \cdot His & 0.000 & 1.107 & Car \cdot Car +His & 120.0 & 120.2 \\ Car \cdot His & 0.000 & 1.007 & Car \cdot Car +His & 120.0 & 120.2 \\ Car \cdot His & 0.950 & 1.0867 & Car \cdot Car +His & 120.0 & 120.2 \\ Car \cdot Lar & 0.950 & 1.0868 & Car \cdot Car +His & 120.0 & 120.1 \\ Car \cdot Lar & 0.950 & 1.0868 & Car \cdot Car +His & 120.0 & 119.7 \\ Car \cdot Car & Lar &$	$C_{29} - C_{31}$	1.379	1.396	$C_3 = N_{12} - C_4$	111.7	114.3
$\begin{array}{ccccccc} {Lab} & 1.326 & 1.323 & {L}^{-n} {L}^{-n} & 1.083 & 1.09.2 \\ {Lab} {Lab} & {L}^{-n} {L}^{-n} & 1.081 & 1.032 & {L}^{-n} {L}^{-n} & 1.00 & 1.194 \\ {Lab} {Lab} & {L}^{-n} {L}^{-n} & 1.00 & 1.194 \\ {Lab} & {L}^{-n} {L}^{-n} & 1.00 & 1.195 & {L}^{-n} {L}^{-n} {L}^{-n} & 1.00 & 1.194 \\ {Lab} & {L}^{-n} {L}^{-n} & 1.00 & 1.107 & {L}^{-n} {L}^{-n} {L}^{-n} & 1.00 & 1.107 \\ {L}^{-n} {L}^{-n} & {L}^{-n} & {L}^{-n} & 1.00 & 1.107 \\ {L}^{-n} {L}^{-n} & {L}^{-n} & {L}^{-n} & 1.00 & 1.107 \\ {L}^{-n} {L}^{-n} & {L}^{-n} & {L}^{-n} & {L}^{-n} & 1.200 & 1.127 \\ {L}^{-n} {L}^{-n} & {L}^{-n} \\ {L}^{-n} {L}^{-n} & {L}^{-n} \\ {L}^{-n} {L}^{-n} & {L}^{-n} \\ {L}^{-n} {L}^{-n} & {L}^$	$C_{35} - C_{36}$	1.522	1.535	$C_3 - N_{12} - H_8$	110.0	109.5
$\begin{array}{c} C_{a} C_{a} C_{a} \\ C_{a} C_{a} C_{a} \\ C_{a} C_{a} \\ C_{b} \\ C$	C <sub>36</sub> -C <sub>39</sub>	1.526	1.533	$C_4 - N_{12} - H_8$	108.8	109.2
$\begin{array}{c} C_{g} - L_{g} & 0.990 & 1.027 & C_{g} - C_{g} - H_{g} & 1.200 & 119.0 \\ C_{g} - H_{g} & 0.990 & 1.027 & C_{g} - C_{g} - H_{g} & 120.0 & 120.3 \\ C_{g} - H_{g} & 1.000 & 1.107 & C_{g} - C_{g} - H_{g} & 120.0 & 119.1 \\ C_{g} - H_{g} & 1.000 & 1.100 & C_{g} - C_{g} - H_{g} & 120.0 & 120.0 \\ C_{g} - H_{g} & 1.000 & 1.100 & C_{g} - C_{g} - H_{g} & 120.0 & 120.0 \\ C_{g} - H_{g} & 0.990 & 1.087 & C_{g} - C_{g} - H_{g} & 120.0 & 120.0 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 119.7 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 119.7 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 119.7 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 118.9 \\ C_{g} - C_{g} & 1.385 & 1.400 & C_{g} - C_{g} - H_{g} & 120.0 & 120.4 \\ C_{g} - C_{g} & 1.385 & 1.400 & C_{g} - C_{g} - H_{g} & 120.0 & 120.4 \\ C_{g} - C_{g} & 1.385 & 1.402 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 120.0 & 120.1 \\ C_{g} - H_{g} & 0.950 & 1.086 & C_{g} - C_{g} - H_{g} & 100.0 & 108.8 \\ C_{g} - H_{g} & 0.990 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 108.8 \\ C_{g} - H_{g} & 0.990 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 108.8 \\ C_{g} - H_{g} & 0.990 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 108.9 \\ C_{g} - H_{g} & 0.990 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 109.1 \\ C_{g} - H_{g} & 0.990 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 109.1 \\ C_{g} - H_{g} & 0.980 & 1.095 & C_{g} - C_{g} - H_{g} & 100.0 & 109.1 \\ C_{g} - C_{g} - C_{g} & 110.8 & 115.7 & C_{g} - C_{g} - H_{g} & 100.0 & 109.1 \\ C_{g} - C_{g} -$	C <sub>39</sub> -C <sub>42</sub>	1.521	1.534	$C_{13} - C_{14} - H_{17}$	120.0	119.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{42} - C_{47}$	1.522	1.532	$C_{16} - C_{14} - H_{17}$	120.0	119.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_2 - H_6$	0.990	1.097	$C_{13} - C_{15} - H_{19}$	120.0	119.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_2-H_7$	0.990	1.092	$C_{18} - C_{15} - H_{19}$	120.0	120.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>3</sub> -H <sub>11</sub>	1.000	1.107	$C_{14} - C_{16} - H_{21}$	120.0	119.7
$\begin{array}{ccccc} -H_{0} & 1.00 & 1.100 & C_{13} - C_{10} - H_{2} & 12.00 & 119.7 \\ C_{14} - H_{17} & 0.951 & 1.007 & C_{10} - H_{22} & 12.00 & 12.00 \\ C_{14} - H_{17} & 0.955 & 1.087 & C_{10} - C_{20} - H_{23} & 12.00 & 12.01 \\ C_{10} - H_{11} & 0.955 & 1.086 & C_{14} - C_{20} - H_{23} & 12.00 & 119.7 \\ C_{10} - H_{21} & 0.955 & 1.086 & C_{24} - C_{24} - H_{24} & 12.00 & 119.7 \\ C_{10} - H_{23} & 0.955 & 1.086 & C_{24} - C_{24} - H_{24} & 12.00 & 119.7 \\ C_{10} - H_{23} & 0.955 & 1.086 & C_{24} - C_{24} - H_{23} & 12.00 & 120.4 \\ C_{24} - C_{26} & 1.385 & 1.400 & C_{29} - C_{24} - H_{23} & 12.00 & 120.4 \\ C_{24} - C_{26} & 1.388 & 1.402 & C_{23} - C_{27} - H_{22} & 12.00 & 120.1 \\ C_{26} - H_{30} & 0.955 & 1.085 & C_{20} - C_{29} - H_{23} & 12.00 & 120.1 \\ C_{26} - H_{31} & 0.955 & 1.085 & C_{29} - C_{29} - H_{33} & 12.00 & 120.0 \\ C_{29} - H_{31} & 0.955 & 1.086 & C_{77} - C_{17} - H_{24} & 12.00 & 120.1 \\ C_{26} - H_{31} & 0.955 & 1.086 & C_{77} - C_{17} - H_{24} & 12.00 & 120.1 \\ C_{26} - H_{31} & 0.955 & 1.086 & C_{77} - C_{17} - H_{24} & 12.00 & 120.1 \\ C_{29} - H_{31} & 0.955 & 1.086 & C_{77} - C_{17} - H_{24} & 12.00 & 120.1 \\ C_{29} - H_{31} & 0.950 & 1.086 & C_{57} - C_{17} - H_{24} & 12.00 & 120.1 \\ C_{26} - H_{31} & 0.950 & 1.086 & C_{57} - C_{51} - H_{34} & 12.00 & 120.2 \\ C_{26} - H_{46} & 0.990 & 1.097 & C_{29} - C_{13} - H_{24} & 120.0 & 120.1 \\ C_{29} - H_{46} & 0.990 & 1.096 & C_{29} - C_{23} - H_{23} & 199.0 & 108.8 \\ C_{20} - H_{40} & 0.990 & 1.099 & C_{20} - C_{20} - H_{23} & 199.0 & 108.1 \\ C_{29} - H_{46} & 0.990 & 1.099 & C_{20} - C_{20} - H_{23} & 199.0 & 109.1 \\ C_{27} - H_{48} & 0.980 & 1.096 & C_{29} - C_{29} - H_{23} & 199.0 & 109.1 \\ C_{27} - H_{26} & 0.980 & 1.096 & C_{29} - C_{29} - H_{23} & 199.0 & 109.1 \\ C_{27} - C_{27} & 110.4 & 11.0 & C_{29} - C_{29} - H_{23} & 199.0 & 109.1 \\ C_{27} - C_{27} & 110.4 & 11.0 & C_{29} - C_{29} - H_{23} & 199.0 & 109.1 \\ C_{27} - C_{27} & 110.4 & 110.0 & C_{29} - C_{29} - H_{23} & 199.0 & 109.1 \\ C_{27} - C_{27} & 110.8 & 111.7 & C_{29} - C_{29} - H_{$	$C_4-H_9$	1.000	1.107	$C_{20} - C_{16} - H_{21}$	120.0	120.1
	$C_5 - H_{10}$	1.000	1.100	$C_{15} - C_{18} - H_{22}$	120.0	119.7
$\begin{array}{c} c_1 + H_{17} & 0.550 & 1.087 & C_1 - C_{27} + H_{23} & 120.0 & 120.2 \\ c_1 + H_{21} & 0.550 & 1.086 & C_{21} - C_{23} + H_{23} & 120.0 & 119.4 \\ c_1 + H_{21} & 0.550 & 1.086 & C_{21} - C_{23} + H_{23} & 120.0 & 119.7 \\ c_2 - H_{23} & 0.550 & 1.086 & C_{21} - C_{23} + H_{23} & 120.0 & 118.9 \\ c_{21} - C_{25} & 1.385 & 1.400 & C_{27} - C_{28} - H_{29} & 120.0 & 119.7 \\ c_{24} - C_{25} & 1.389 & 1.402 & C_{21} - H_{22} & 120.0 & 119.7 \\ c_{23} - H_{23} & 0.550 & 1.086 & C_{21} - C_{29} - H_{22} & 120.0 & 119.7 \\ c_{23} - H_{23} & 0.550 & 1.087 & C_{21} - C_{27} - H_{22} & 120.0 & 119.7 \\ c_{23} - H_{29} & 0.550 & 1.085 & C_{21} - C_{29} + H_{31} & 120.0 & 119.7 \\ c_{27} - H_{22} & 0.550 & 1.086 & C_{21} - C_{29} - H_{31} & 120.0 & 119.7 \\ c_{29} - H_{21} & 0.550 & 1.086 & C_{21} - C_{21} - C_{29} & 119.7 & 119.6 \\ c_{31} - H_{34} & 0.550 & 1.086 & C_{27} - C_{31} - C_{39} & 119.7 & 119.6 \\ c_{31} - H_{34} & 0.590 & 1.096 & C_{5} - C_{51} - H_{54} & 120.0 & 120.1 \\ c_{35} - H_{37} & 0.990 & 1.097 & C_{29} - H_{31} & 120.0 & 120.1 \\ c_{35} - H_{37} & 0.990 & 1.096 & C_{5} - C_{53} - H_{37} & 109.0 & 108.8 \\ c_{37} - H_{41} & 0.090 & 1.096 & C_{5} - C_{53} - H_{37} & 109.0 & 108.9 \\ c_{37} - H_{43} & 0.990 & 1.096 & C_{37} - C_{37} - H_{34} & 109.0 & 108.9 \\ c_{37} - H_{43} & 0.990 & 1.096 & C_{37} - C_{37} - H_{34} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.490 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.490 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.490 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.490 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.490 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - C_{47} & 0.990 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - C_{47} & 0.990 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - C_{47} & 0.990 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.1 \\ c_{47} - C_{47} & 0.990 & 1.096 & C_{37} - C_{37} - H_{31} & 109.0 & 109.$	$H_8 - N_{12}$	0.911	1.017	$C_{20} - C_{18} - H_{22}$	120.0	120.0
$\begin{array}{c} c_3-H_{19} & 0.950 & 1.086 & C_3-C_{32}-H_{38} & 120.0 & 120.1 \\ C_{10}-H_{21} & 0.950 & 1.086 & C_3-C_{32}-H_{38} & 120.0 & 119.7 \\ C_{10}-H_{22} & 0.950 & 1.086 & C_3-C_{32}-H_{38} & 120.0 & 119.7 \\ C_{10}-H_{21} & 0.950 & 1.086 & C_3-C_{32}-H_{30} & 120.0 & 120.4 \\ C_{32}-C_{35} & 1.385 & 1.400 & C_{32}-C_{32}-H_{30} & 120.0 & 119.7 \\ C_{32}-H_{32} & 0.950 & 1.087 & C_{31}-C_{32}-H_{31} & 120.0 & 119.7 \\ C_{33}-H_{32} & 0.950 & 1.087 & C_{31}-C_{32}-H_{33} & 120.0 & 119.7 \\ C_{33}-H_{32} & 0.950 & 1.085 & C_{31}-C_{32}-H_{33} & 120.0 & 120.1 \\ C_{32}-H_{32} & 0.950 & 1.086 & C_{31}-C_{32}-H_{33} & 120.0 & 120.1 \\ C_{32}-H_{31} & 0.950 & 1.086 & C_{31}-C_{32}-H_{33} & 120.0 & 120.1 \\ C_{32}-H_{31} & 0.950 & 1.086 & C_{31}-C_{32}-H_{33} & 120.0 & 120.1 \\ C_{33}-H_{34} & 0.950 & 1.086 & C_{31}-C_{31}-H_{34} & 120.0 & 120.1 \\ C_{33}-H_{34} & 0.950 & 1.086 & C_{31}-C_{31}-H_{34} & 120.0 & 120.1 \\ C_{33}-H_{34} & 0.950 & 1.086 & C_{31}-C_{31}-H_{34} & 120.0 & 120.1 \\ C_{33}-H_{34} & 0.990 & 1.097 & C_{32}-C_{31}-H_{34} & 120.0 & 108.8 \\ C_{33}-H_{34} & 0.990 & 1.096 & C_{31}-C_{32}-H_{33} & 109.0 & 108.8 \\ C_{33}-H_{34} & 0.990 & 1.100 & C_{32}-C_{32}-H_{38} & 109.0 & 108.9 \\ C_{33}-H_{34} & 0.990 & 1.098 & C_{31}-C_{32}-H_{38} & 109.0 & 109.1 \\ C_{33}-H_{34} & 0.990 & 1.098 & C_{31}-C_{32}-H_{38} & 109.0 & 109.1 \\ C_{33}-H_{34} & 0.990 & 1.099 & C_{31}-C_{32}-H_{38} & 109.0 & 109.1 \\ C_{33}-H_{34} & 0.980 & 1.096 & C_{31}-C_{32}-H_{38} & 109.0 & 109.1 \\ C_{33}-H_{34} & 0.980 & 1.096 & C_{33}-C_{33}-H_{38} & 109.0 & 109.1 \\ C_{37}-H_{30} & 0.980 & 1.096 & C_{32}-C_{32}-H_{34} & 109.0 & 109.1 \\ C_{37}-H_{30} & 0.980 & 1.096 & C_{32}-C_{32}-H_{44} & 109.0 & 109.1 \\ C_{37}-H_{30} & 0.980 & 1.096 & C_{32}-C_{32}-H_{44} & 109.0 & 109.1 \\ C_{37}-H_{30} & 0.980 & 1.096 & C_{33}-C_{33}-H_{33} & 109.0 & 109.1 \\ C_{37}-H_{30} & 0.980 & 1.096 & C_{32}-C_{33}-H_{44} & 109.0 & 109.1 \\ C_{37}-C_{35} & 116.0 & 115.1 & H_{32}-C_{33}-H_{44} & 109.0 & 109.1 \\ C_{37}-C_{35} & 112.3 & 112.8 & C_{33}-C_{33}-H_{44} & 109.0 & 109$	C <sub>14</sub> -H <sub>17</sub>	0.950	1.087	$C_{16} - C_{20} - H_{23}$	120.0	120.2
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$C_{15}-H_{19}$	0.950	1.086	$C_{18} - C_{20} - H_{23}$	120.0	120.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>16</sub> -H <sub>21</sub>	0.950	1.086	$C_{24} - C_{25} - H_{28}$	120.0	119.4
$\begin{array}{c} C_{2n}-R_{2n} & 0.950 & 1.086 & C_{2n}-C_{3n} & 12.00 & 118.9 \\ C_{3n}-C_{5n} & 1.385 & 1.400 & C_{2n}-C_{5n}-H_{3n} & 12.00 & 113.7 \\ C_{5n}-H_{5n} & 0.950 & 1.087 & C_{2n}-C_{2n}-H_{3n} & 12.00 & 113.7 \\ C_{5n}-H_{5n} & 0.950 & 1.087 & C_{2n}-C_{2n}-H_{3n} & 12.00 & 113.7 \\ C_{5n}-H_{5n} & 0.950 & 1.086 & C_{2n}-C_{2n}-H_{3n} & 12.00 & 120.1 \\ C_{5n}-H_{5n} & 0.950 & 1.086 & C_{2n}-C_{2n}-H_{3n} & 12.00 & 120.1 \\ C_{5n}-H_{5n} & 0.950 & 1.086 & C_{2n}-C_{2n}-H_{3n} & 12.00 & 120.1 \\ C_{5n}-H_{5n} & 0.950 & 1.086 & C_{2n}-C_{2n}-H_{3n} & 120.0 & 120.1 \\ C_{5n}-H_{5n} & 0.950 & 1.086 & C_{2n}-C_{2n}-H_{3n} & 120.0 & 120.1 \\ C_{5n}-H_{5n} & 0.990 & 1.097 & C_{2n}-C_{1n}+H_{4n} & 120.0 & 120.1 \\ C_{5n}-H_{5n} & 0.990 & 1.096 & C_{5n}-C_{3n}-H_{3n} & 109.0 & 108.8 \\ C_{5n}-H_{4n} & 0.990 & 1.095 & C_{n}-C_{2n}-H_{3n} & 109.0 & 108.9 \\ C_{5n}-H_{4n} & 0.990 & 1.096 & C_{5n}-C_{5n}-H_{3n} & 109.0 & 108.9 \\ C_{5n}-H_{4n} & 0.990 & 1.099 & H_{7n}-C_{5n}-H_{3n} & 109.0 & 108.9 \\ C_{5n}-H_{4n} & 0.990 & 1.099 & H_{7n}-C_{5n}-H_{3n} & 109.0 & 108.9 \\ C_{2n}-H_{4n} & 0.990 & 1.099 & C_{5n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-H_{4n} & 0.990 & 1.099 & C_{5n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-H_{4n} & 0.990 & 1.099 & C_{5n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-H_{4n} & 0.980 & 1.099 & C_{5n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-H_{4n} & 0.980 & 1.099 & C_{5n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-C_{2n} & 116.0 & 115.1 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.1 \\ C_{2n}-C_{2n} & 116.0 & 115.1 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 116.0 & 115.1 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 110.8 & 111.7 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 110.8 & 111.7 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 110.8 & 111.7 & C_{2n}-C_{5n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 100.6 & 115.1 & H_{2n}-C_{2n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 100.6 & 116.7 & H_{2n}-C_{2n}-H_{4n} & 109.0 & 109.2 \\ C_{2n}-C_{2n} & 100.6 & 116.7 & H_{2n}-C_{2n}-H_{4n} & 109.$	C <sub>18</sub> -H <sub>22</sub>	0.950	1.086	$C_{27} - C_{25} - H_{28}$	120.0	119.7
$\begin{array}{cccc} C_{2a} - C_{2b} & 1.385 & 1.400 & C_{2a} - C_{2b} & 12.00 & 120.1 \\ C_{2a} - C_{2b} & 13.89 & 1.402 & C_{2b} - C_{2b} & 120.0 & 120.1 \\ C_{2a} - H_{2b} & 0.950 & 1.087 & C_{1a} - C_{2b} + H_{2b} & 120.0 & 120.1 \\ C_{2a} - H_{2b} & 0.950 & 1.085 & C_{2a} - C_{2b} + H_{2b} & 120.0 & 120.1 \\ C_{2a} - H_{2b} & 0.950 & 1.086 & C_{2a} - C_{2b} + H_{2b} & 120.0 & 120.1 \\ C_{2a} - H_{2b} & 0.950 & 1.086 & C_{2b} - C_{2b} & 119.7 & 119.6 \\ C_{2a} - H_{2b} & 0.950 & 1.086 & C_{2b} - C_{2b} & 119.7 & 119.6 \\ C_{3a} - H_{3b} & 0.950 & 1.086 & C_{2b} - C_{1b} + H_{2b} & 120.0 & 120.1 \\ C_{3a} - H_{3b} & 0.990 & 1.097 & C_{2b} - C_{1b} + H_{2b} & 120.0 & 120.1 \\ C_{3a} - H_{3b} & 0.990 & 1.095 & C_{2b} - C_{1b} + H_{2b} & 120.0 & 120.2 \\ C_{3a} - H_{4b} & 0.990 & 1.095 & C_{2b} - C_{3a} + H_{3b} & 109.0 & 108.8 \\ C_{3a} - H_{4b} & 0.990 & 1.000 & C_{2b} - C_{2b} + H_{3b} & 109.0 & 108.1 \\ C_{2a} - H_{4b} & 0.990 & 1.009 & H_{2b} - C_{2b} - H_{3b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.990 & 1.099 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.990 & 1.099 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.980 & 1.096 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.980 & 1.095 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.980 & 1.095 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{4b} & 0.980 & 1.095 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - H_{2b} & 0.980 & 1.095 & C_{2b} - C_{2b} - H_{2b} & 109.0 & 100.1 \\ C_{2a} - C_{2c} - C_{2c} & 111.4 & 110.0 & C_{2a} - C_{2b} - H_{2b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 111.4 & 110.0 & C_{2a} - C_{2b} - H_{4b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 110.8 & 111.7 & C_{2b} - C_{2b} - H_{4b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 110.8 & 111.7 & C_{2b} - C_{2b} - H_{4b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 110.8 & 111.7 & C_{2b} - C_{2b} - H_{4b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 110.8 & 111.7 & C_{2b} - C_{2b} - H_{4b} & 109.0 & 109.1 \\ C_{2c} - C_{2c} & 111.4 & 110.0 & C_{2b} - C_{2b} - H_{4b} & $	C <sub>20</sub> -H <sub>23</sub>	0.950	1.086	$C_{24} - C_{26} - H_{30}$	120.0	118.9
$\begin{array}{cccc} C_{2a}-C_{2a} & -H_{2a} & 0.050 & 1.087 & C_{2a}-C_{2a}-H_{2a} & 12.0. & 119.7 \\ C_{2a}+H_{3b} & 0.050 & 1.085 & C_{3a}-C_{2a}-H_{3b} & 12.0. & 120.1 \\ C_{2a}+H_{31} & 0.050 & 1.086 & C_{31}-C_{2a}-H_{3b} & 120.0 & 120.0 \\ C_{2a}+H_{31} & 0.050 & 1.086 & C_{31}-C_{31}-H_{3b} & 120.0 & 120.1 \\ C_{3a}+H_{31} & 0.050 & 1.086 & C_{2a}-C_{31}-H_{3b} & 120.0 & 120.1 \\ C_{3a}+H_{31} & 0.050 & 1.086 & C_{2a}-C_{31}-H_{3b} & 120.0 & 120.1 \\ C_{3a}+H_{31} & 0.050 & 1.086 & C_{2a}-C_{31}-H_{3b} & 120.0 & 120.2 \\ C_{3a}-H_{30} & 0.099 & 1.097 & C_{2a}-C_{31}-H_{3b} & 120.0 & 120.2 \\ C_{3a}-H_{30} & 0.0990 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 108.8 \\ C_{3a}-H_{41} & 0.0990 & 1.100 & C_{3a}-C_{3a}-H_{3a} & 109.0 & 108.9 \\ C_{3a}-H_{41} & 0.0990 & 1.099 & C_{3a}-C_{3a}-H_{3a} & 109.0 & 108.9 \\ C_{3a}-H_{41} & 0.990 & 1.099 & C_{3a}-C_{3a}-H_{3a} & 109.0 & 108.1 \\ C_{3a}-H_{4a} & 0.990 & 1.099 & C_{3a}-C_{3a}-H_{3a} & 108.0 & 107.0 \\ C_{aa}-H_{4a} & 0.990 & 1.099 & C_{3a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4a} & 0.980 & 1.096 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4a} & 0.980 & 1.096 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4b} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4b} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4b} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4b} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{4b} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-H_{ab} & 0.980 & 1.095 & C_{2a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-C_{ab} & 111.4 & 110.0 & C_{3a}-C_{3a}-H_{3a} & 109.0 & 109.1 \\ C_{aa}-C_{ab} & 111.4 & 110.0 & C_{ab}-C_{aa}-H_{ab} & 109.0 & 109.4 \\ C_{aa}-C_{ab} & 111.2 & C_{ab}-C_{aa}-H_{ab} & 109.0 & 109.2 \\ C_{aa}-C_{aa}-C_{ab} & 110.3 & 111.7 & C_{ab}-C_{aa}-H_{ab} & 109.0 & 109.1 \\ C_{aa}-C_{aa}-C_{ab} & 110.3 & 111.7 & C_{ab}-C_{aa}-H_{ab} & 109.0 & 109.1 \\ C_{aa}-C_{aa}-C_{ab} & 110.3 & 112.8 & C_{aa}-C_{aa}-H_{ab} & 109.0 & 109.1 \\ C_{aa}-C_{aa}-C_{ab} &$	C <sub>24</sub> -C <sub>25</sub>	1.385	1.400	$C_{29} - C_{26} - H_{30}$	120.0	120.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{24} - C_{26}$	1.389	1.402	$C_{25} - C_{27} - H_{32}$	120.0	119.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>25</sub> -H <sub>28</sub>	0.950	1.087	$C_{31} - C_{27} - H_{32}$	120.0	120.1
$\begin{array}{ccccc} c_2 - H_{32} & 0.950 & 1.086 & C_1 - C_9 + H_{33} & 120.0 & 120.0 \\ c_{30} + H_{31} & 0.950 & 1.086 & C_1 - C_1 - H_{34} & 120.0 & 120.1 \\ c_{31} + H_{34} & 0.950 & 1.086 & C_2 - C_{31} - H_{34} & 120.0 & 120.1 \\ c_{35} + H_{36} & 0.990 & 1.097 & C_9 - C_{11} - H_{34} & 120.0 & 120.2 \\ c_{35} + H_{36} & 0.990 & 1.095 & C_7 - C_{33} + H_{37} & 109.0 & 108.8 \\ c_{36} - H_{41} & 0.990 & 1.095 & C_7 - C_{33} - H_{37} & 109.0 & 108.9 \\ c_{39} - H_{41} & 0.990 & 1.100 & C_{36} - C_{35} - H_{38} & 109.0 & 108.9 \\ c_{39} - H_{41} & 0.990 & 1.009 & H_{17} - C_{55} - H_{38} & 109.0 & 108.9 \\ c_{39} - H_{41} & 0.990 & 1.009 & C_{36} - C_{35} - H_{36} & 109.0 & 100.2 \\ c_{2} - H_{45} & 0.990 & 1.009 & C_{36} - C_{35} - H_{40} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & C_{36} - C_{35} - H_{40} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & C_{36} - C_{53} - H_{37} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & C_{36} - C_{35} - H_{38} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & C_{36} - C_{53} - H_{38} & 109.0 & 109.1 \\ c_{47} - H_{49} & 0.980 & 1.095 & C_{36} - C_{53} - H_{38} & 109.0 & 109.1 \\ c_{47} - H_{49} & 0.980 & 1.095 & C_{36} - C_{53} - H_{38} & 109.0 & 109.1 \\ c_{47} - H_{49} & 0.980 & 1.095 & C_{36} - C_{53} - H_{38} & 109.0 & 109.1 \\ c_{47} - C_{45} & 111.4 & 110.0 & C_{36} - C_{53} - H_{41} & 109.0 & 109.1 \\ c_{47} - C_{45} & 111.4 & 110.0 & C_{36} - C_{39} - H_{41} & 109.0 & 109.2 \\ c_{5} - C_{4} & 10.8 & 111.7 & C_{46} - C_{29} - H_{43} & 109.0 & 109.2 \\ c_{5} - C_{4} & 10.9 & 107.6 & C_{29} - C_{29} - H_{43} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{4} & 109.6 & 107.6 & C_{29} - C_{9} - H_{44} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{5} & 107.0 & 112.4 & H_{43} - C_{59} - H_{44} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{5} & 107.0 & 112.4 & H_{45} - C_{47} - H_{16} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{5} & 107.0 & 118.7 & H_{45} - C_{47} - H_{49} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{5} & 109.0 & 118.7 & H_{45} - C_{47} - H_{46} & 109.0 & 109.1 \\ c_{4} - C_{5} - C_{5} & 109.0 & 118.7 $	C <sub>26</sub> -H <sub>30</sub>	0.950	1.085	C <sub>26</sub> -C <sub>29</sub> -H <sub>33</sub>	120.0	119.7
	C <sub>27</sub> -H <sub>32</sub>	0.950	1.086	C <sub>31</sub> -C <sub>29</sub> -H <sub>33</sub>	120.0	120.0
	C <sub>29</sub> -H <sub>33</sub>	0.950	1.086	$C_{27} - C_{31} - C_{29}$	119.7	119.6
	C <sub>31</sub> -H <sub>34</sub>	0.950	1.086	$C_{27} - C_{31} - H_{34}$	120.0	120.1
$\begin{array}{ccccc} c_3 - H_{36} & 0.990 & 1.096 & c_5 - C_{35} - H_{37} & 109.0 & 108.8 \\ c_{36} - H_{40} & 0.990 & 1.095 & c_5 - C_{35} - H_{38} & 109.0 & 108.9 \\ c_{36} - H_{41} & 0.990 & 1.100 & c_{36} - C_{35} - H_{38} & 109.0 & 108.9 \\ c_{39} - H_{43} & 0.990 & 1.009 & H_{37} - C_{35} - H_{38} & 109.0 & 108.9 \\ c_{39} - H_{44} & 0.990 & 1.099 & H_{37} - C_{35} - H_{38} & 109.0 & 109.1 \\ c_{27} - H_{45} & 0.990 & 1.099 & c_{35} - C_{36} - H_{41} & 109.0 & 109.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & c_{39} - C_{36} - H_{41} & 109.0 & 109.4 \\ c_{47} - H_{48} & 0.980 & 1.096 & c_{39} - C_{36} - H_{41} & 109.0 & 109.4 \\ c_{47} - H_{48} & 0.980 & 1.096 & c_{36} - C_{35} - H_{37} & 109.0 & 108.1 \\ c_{47} - H_{48} & 0.980 & 1.096 & c_{36} - C_{37} - H_{37} & 109.0 & 108.9 \\ Bond angle (^{\circ)} & c_{39} - C_{36} - H_{41} & 109.0 & 109.0 & 109.4 \\ c_{2} - c_{5} & 116.0 & 115.1 & H_{40} - C_{36} - H_{41} & 108.0 & 106.7 \\ c_{4} - c_{5} & 111.4 & 110.0 & c_{36} - C_{39} - H_{43} & 109.0 & 109.4 \\ c_{2} - c_{5} - c_{5} & 111.1 & 110.8 & 111.7 & c_{36} - c_{39} - H_{43} & 109.0 & 109.2 \\ c_{5} - c_{4} - c_{13} & 112.3 & 112.8 & c_{42} - c_{39} - H_{44} & 109.0 & 109.2 \\ c_{5} - c_{4} - c_{13} & 112.3 & 112.8 & c_{42} - c_{39} - H_{44} & 108.0 & 106.7 \\ c_{4} - c_{5} - c_{5} & 107.0 & 112.4 & H_{4} - C_{39} - H_{44} & 108.0 & 106.0 \\ c_{4} - c_{5} - c_{5} & 107.0 & 112.4 & H_{4} - C_{39} - H_{44} & 108.0 & 106.0 \\ c_{4} - c_{5} - c_{5} & 102.1 & 113.9 & c_{39} - c_{4} - H_{46} & 108.0 & 105.9 \\ c_{4} - c_{13} - c_{14} & 120.9 & 120.7 & c_{39} - c_{4} + H_{6} & 108.0 & 105.9 \\ c_{4} - c_{13} - c_{14} & 109.0 & 118.7 & H_{4} - c_{4} - c_{47} & 109.0 & 109.1 \\ c_{1} - c_{1} - c_{16} & 120.8 & H_{46} - c_{4} - c_{47} & 109.0 & 109.4 \\ c_{3} - c_{15} - c_{18} & 120.8 & H_{46} - c_{4} - c_{47} & 109.0 & 109.4 \\ c_{3} - c_{14} - c_{16} & 120.8 & H_{46} - c_{4} - c_{47} & 109.0 & 107.4 \\ c_{3} - c_{5} - c_{5} & 112.1 & 120.9 & C_{4} - c_{4} - H_{49} & 109.0 & 111.1 \\ c_{4} - c_{16} - c_{20} & 119.6 & 120.0 & c_{4} - c_{4} - H_{49} & 109.0 &$	C <sub>35</sub> -H <sub>37</sub>	0.990	1.097	$C_{29} - C_{31} - H_{34}$	120.0	120.2
$ \begin{array}{ccccc} \hline C_{36} - H_{40} & 0.990 & 1.095 & C_{5} - C_{35} - H_{38} & 109.0 & 108.9 \\ C_{39} - H_{41} & 0.990 & 1.100 & C_{36} - C_{35} - H_{37} & 109.0 & 108.9 \\ C_{39} - H_{43} & 0.990 & 1.099 & H_{37} - C_{35} + H_{38} & 108.0 & 107.0 \\ C_{42} - H_{44} & 0.990 & 1.099 & H_{37} - C_{35} + H_{38} & 108.0 & 107.0 \\ C_{42} - H_{45} & 0.990 & 1.099 & C_{35} - C_{36} - H_{41} & 109.0 & 109.1 \\ C_{47} - H_{48} & 0.980 & 1.096 & C_{39} - C_{35} - H_{41} & 109.0 & 109.1 \\ C_{47} - H_{48} & 0.980 & 1.096 & C_{39} - C_{35} - H_{41} & 109.0 & 109.1 \\ C_{47} - H_{48} & 0.980 & 1.096 & C_{39} - C_{35} - H_{41} & 109.0 & 109.1 \\ C_{47} - H_{48} & 0.980 & 1.095 & C_{36} - C_{35} + H_{31} & 109.0 & 108.9 \\ C_{47} - H_{48} & 0.980 & 1.095 & C_{36} - C_{35} + H_{31} & 109.0 & 108.9 \\ C_{47} - C_{5} & 116.0 & 115.1 & H_{40} - C_{59} - H_{41} & 108.0 & 106.7 \\ C_{2} - C_{2} - C_{5} & 116.0 & 115.1 & H_{40} - C_{59} - H_{41} & 109.0 & 109.4 \\ C_{2} - C_{1} - C_{5} & 111.4 & 110.0 & C_{36} - C_{39} - H_{41} & 109.0 & 109.4 \\ C_{2} - C_{1} - C_{5} & 111.4 & 110.0 & C_{36} - C_{39} - H_{41} & 109.0 & 109.2 \\ C_{5} - C_{4} - C_{13} & 112.3 & 112.8 & C_{42} - C_{39} - H_{44} & 109.0 & 109.2 \\ C_{1} - C_{5} - C_{4} & 109.6 & 107.6 & C_{42} - C_{39} - H_{44} & 109.0 & 109.2 \\ C_{1} - C_{5} - C_{4} & 109.6 & 107.6 & C_{42} - C_{49} - H_{46} & 109.0 & 109.1 \\ C_{4} - C_{13} - C_{15} & 120.4 & 120.7 & C_{39} - C_{42} - H_{46} & 109.0 & 109.1 \\ C_{4} - C_{13} - C_{15} & 120.4 & 120.5 & H_{4} - C_{42} - C_{47} & 109.0 & 109.1 \\ C_{4} - C_{13} - C_{15} & 120.4 & 120.5 & H_{4} - C_{42} - C_{47} & 109.0 & 109.1 \\ C_{4} - C_{13} - C_{15} & 120.4 & 120.5 & H_{4} - C_{42} - C_{47} & 109.0 & 109.4 \\ C_{3} - C_{15} - C_{18} & 120.8 & 120.6 & C_{42} - C_{47} - H_{48} & 109.0 & 109.4 \\ C_{3} - C_{15} - C_{18} & 120.8 & 120.6 & C_{42} - C_{47} - H_{48} & 109.0 & 111.1 \\ C_{4} - C_{15} - C_{18} & 120.8 & 120.6 & C_{42} - C_{47} - H_{49} & 109.0 & 111.1 \\ C_{4} - C_{15} - C_{26} & 120.8 & 120.0 & C_{42} - C_{47} - H_{48} & 109.0 & 111.1 \\ C_{4} - C_{$	C35-H38	0.990	1.096	C5-C35-H37	109.0	108.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>36</sub> -H <sub>40</sub>	0.990	1.095	C5-C35-H38	109.0	108.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{36} - H_{41}$	0.990	1.100	C <sub>36</sub> -C <sub>35</sub> -H <sub>37</sub>	109.0	109.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>30</sub> -H <sub>43</sub>	0.990	1.100	C <sub>36</sub> -C <sub>35</sub> -H <sub>38</sub>	109.0	108.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C <sub>39</sub> -H <sub>44</sub>	0.990	1.099	$H_{37} - C_{35} - H_{38}$	108.0	107.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C42-H45	0.990	1 098	C25-C26-H40	109.0	109.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C42-H46	0.990	1 099	$C_{25} - C_{26} - H_{41}$	109.0	109.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C47-H49	0.980	1 096	$C_{20} - C_{26} - H_{40}$	109.0	109.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C47 H48	0.980	1 096	$C_{39} = C_{36} = H_{37}$	109.0	109.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C47-H51	0.980	1.095	Cac-Cas-Han	109.0	108.9
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Bond angle (°)	0.500	1.035	Coo=Coo=H44	109.0	109.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		116.0	115 1		105.0	105.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$c_2 - c_1 - c_3$	111.0	110.0	$\Gamma_{140} - C_{36} - \Gamma_{141}$	100.0	100.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_1 - C_2 - C_3$	111.4	111.7		109.0	109.4
$\begin{array}{cccccccc} c_1c_5-c_4& 109.6& 107.6& c_42-c_39-143& 109.0& 109.1\\ c_1-c_5-c_35& 107.0& 112.4& H_{43}-c_{39}-H_{44}& 109.0& 109.1\\ c_4-c_5-c_{35}& 112.1& 113.9& c_{39}-c_{42}-H_{45}& 109.0& 109.1\\ c_4-c_{13}-c_{14}& 120.9& 120.7& c_{39}-c_{42}-H_{46}& 109.0& 109.2\\ c_4-c_{13}-c_{15}& 120.4& 120.5& H_{45}-c_{42}-H_{46}& 108.0& 105.9\\ c_{14}-c_{13}-c_{15}& 109.0& 118.7& H_{45}-c_{42}-c_{47}& 109.0& 109.4\\ c_{13}-c_{14}-c_{16}& 120.9& 120.8& H_{46}-c_{42}-c_{47}& 109.0& 109.4\\ c_{13}-c_{15}-c_{18}& 120.8& 120.6& c_{42}-c_{47}-H_{48}& 109.0& 111.1\\ c_{14}-c_{16}-c_{20}& 119.6& 120.0& c_{42}-c_{47}-H_{49}& 109.0& 111.2\\ c_{15}-c_{18}-c_{20}& 120.3& 120.2& c_{42}-c_{47}-H_{51}& 109.0& 111.5\\ c_{16}-c_{20}-c_{18}& 119.9& 119.6& H_{48}-c_{47}-H_{51}& 109.0& 107.4\\ c_{3}-c_{24}-c_{25}& 119.9& 120.2& H_{48}-c_{47}-H_{51}& 109.0& 107.6\\ c_{3}-c_{24}-c_{26}& 118.8& 118.8& Dihedral (^{\circ})\\ c_{25}-c_{24}-c_{26}& 118.8& 118.8& Dihedral (^{\circ})\\ c_{24}-c_{25}-c_{27}& 120.3& 120.7& c_{2}-c_{N12}-C_{4}& -66.82& -62.88\\ c_{24}-c_{26}-c_{29}& 120.8& 120.5& c_{24}-c_{3}-N_{12}-c_{4}& 172.32& 174.49\\ \end{array}$	$C_2 - C_3 - C_{24}$	110.0	111.7	$C_{36}-C_{39}-H_{44}$	109.0	109.2
$\begin{array}{ccccccc} c_1-c_5-c_4 & 109.0 & 107.0 & 12.4 & 143-c_{39}-r_{44} & 109.0 & 109.1 \\ c_1-c_5-c_{35} & 107.0 & 112.4 & H_{43}-c_{39}-H_{44} & 108.0 & 106.0 \\ c_4-c_5-c_{35} & 112.1 & 113.9 & c_{39}-c_42-H_{45} & 109.0 & 109.1 \\ c_4-c_{13}-c_{15} & 120.4 & 120.5 & H_{45}-c_{42}-H_{46} & 108.0 & 105.9 \\ c_{14}-c_{13}-c_{15} & 109.0 & 118.7 & H_{45}-c_{42}-c_{47} & 109.0 & 109.4 \\ c_{13}-c_{14}-c_{16} & 120.9 & 120.8 & H_{46}-c_{42}-c_{47} & 109.0 & 109.4 \\ c_{13}-c_{15}-c_{18} & 120.8 & 120.6 & c_{42}-c_{47}-H_{48} & 109.0 & 111.1 \\ c_{15}-c_{18}-c_{20} & 119.6 & 120.0 & c_{42}-c_{47}-H_{48} & 109.0 & 111.2 \\ c_{15}-c_{18}-c_{20} & 120.3 & 120.2 & c_{42}-c_{47}-H_{49} & 109.0 & 111.2 \\ c_{15}-c_{18}-c_{20} & 120.3 & 120.2 & c_{42}-c_{47}-H_{51} & 109.0 & 111.5 \\ c_{16}-c_{20}-c_{18} & 119.9 & 119.6 & H_{48}-c_{47}-H_{51} & 109.0 & 107.4 \\ c_{3}-c_{24}-c_{25} & 119.9 & 120.2 & H_{48}-c_{47}-H_{51} & 109.0 & 107.6 \\ c_{25}-c_{24}-c_{26} & 118.8 & 118.8 & Dihedral (^{\circ}) \\ c_{25}-c_{24}-c_{26} & 120.3 & 120.7 & c_{2}-c_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ c_{24}-c_{26}-c_{29} & 120.8 & 120.5 & c_{24}-c_{3}-N_{12}-C_{4} & 172.32 & 174.49 \\ \end{array}$	$C_5 - C_4 - C_{13}$	100.6	107.6	$C_{42} - C_{39} - \Gamma_{43}$	109.0	109.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$c_1 - c_5 - c_4$	107.0	112.4	$C_{42} - C_{39} - \Pi_{44}$	109.0	109.1
$\begin{array}{cccccccc} L_4 - C_5 - C_{35} & 112.1 & 113.9 & C_{39} - C_{42} - H_{45} & 109.0 & 109.1 \\ C_4 - C_{13} - C_{14} & 120.9 & 120.7 & C_{39} - C_{42} - H_{46} & 109.0 & 109.2 \\ C_4 - C_{13} - C_{15} & 120.4 & 120.5 & H_{45} - C_{42} - H_{46} & 108.0 & 105.9 \\ C_{13} - C_{14} - C_{16} & 120.9 & 118.7 & H_{45} - C_{42} - C_{47} & 109.0 & 109.4 \\ C_{13} - C_{13} - C_{16} & 120.8 & 120.6 & C_{42} - C_{47} - H_{48} & 109.0 & 111.1 \\ C_{14} - C_{16} - C_{20} & 119.6 & 120.0 & C_{42} - C_{47} - H_{49} & 109.0 & 111.2 \\ C_{15} - C_{18} & 120.3 & 120.2 & C_{42} - C_{47} - H_{49} & 109.0 & 111.2 \\ C_{15} - C_{18} - C_{20} - C_{18} & 119.9 & 119.6 & H_{48} - C_{47} - H_{51} & 109.0 & 111.5 \\ C_{16} - C_{20} - C_{18} & 119.9 & 120.2 & H_{48} - C_{47} - H_{51} & 109.0 & 107.4 \\ C_{3} - C_{24} - C_{25} & 119.9 & 120.2 & H_{48} - C_{47} - H_{51} & 109.0 & 107.6 \\ C_{25} - C_{24} - C_{26} & 118.8 & 118.8 & Dihedral (°) \\ C_{25} - C_{24} - C_{26} & 120.3 & 120.7 & C_{2} - C_{17} - M_{27} & -66.82 & -62.88 \\ C_{24} - C_{26} - C_{29} & 120.8 & 120.5 & C_{24} - C_{3} - N_{12} - C_{4} & 172.32 & 174.49 \\ \end{array}$	$C_1 - C_5 - C_{35}$	107.0	112.4	$H_{43}-C_{39}-H_{44}$	108.0	106.0
$\begin{array}{ccccccc} L_4 - L_1 - L_1 & 120.9 & 120.7 & L_{39} - L_{42} - H_{46} & 109.0 & 109.2 \\ L_4 - L_{13} - L_{15} & 120.4 & 120.5 & H_{45} - L_{42} - H_{46} & 108.0 & 105.9 \\ L_1 - L_{14} - L_{15} - L_{14} - L_{16} & 120.9 & 118.7 & H_{45} - L_{42} - L_{47} & 109.0 & 109.4 \\ L_{13} - L_{14} - L_{16} & 120.9 & 120.8 & H_{46} - L_{42} - L_{47} & 109.0 & 109.4 \\ L_{13} - L_{15} - L_{18} & 120.8 & 120.6 & L_{42} - L_{47} - H_{48} & 109.0 & 111.1 \\ L_{14} - L_{16} - L_{20} & 119.6 & 120.0 & L_{42} - L_{47} - H_{49} & 109.0 & 111.2 \\ L_{15} - L_{18} - L_{20} & 120.3 & 120.2 & L_{42} - L_{47} - H_{49} & 109.0 & 111.5 \\ L_{16} - L_{20} - L_{18} & 119.9 & 119.6 & H_{48} - L_{47} - H_{49} & 109.0 & 107.4 \\ L_{3} - L_{24} - L_{25} & 119.9 & 120.2 & H_{48} - L_{47} - H_{49} & 109.0 & 107.4 \\ L_{3} - L_{24} - L_{25} & 119.9 & 120.2 & H_{48} - L_{47} - H_{51} & 109.0 & 107.6 \\ L_{25} - L_{26} - L_{26} & 118.8 & 118.8 & Dihedral (°) & L_{25} - L_{27} - L_{26} & 120.3 & 120.7 & L_{27} - L_{27} - L_{26} - L_{26} & -62.88 \\ L_{24} - L_{26} - L_{29} & 120.8 & 120.5 & L_{24} - L_{27} - L_{24} & -66.82 & -62.88 \\ L_{24} - L_{26} - L_{29} & 120.8 & 120.5 & L_{24} - L_{27} - L_{24} & 172.32 & 174.49 \\ \end{array}$	$C_4 - C_5 - C_{35}$	112.1	113.9	$C_{39} - C_{42} - H_{45}$	109.0	109.1
$\begin{array}{ccccccc} L_4 - C_{13} - C_{15} & 120.4 & 120.5 & H_{45} - C_{42} - H_{46} & 108.0 & 105.9 \\ C_{14} - C_{13} - C_{15} & 109.0 & 118.7 & H_{45} - C_{42} - C_{47} & 109.0 & 109.4 \\ C_{13} - C_{15} - C_{18} & 120.8 & 120.6 & C_{42} - C_{47} & 109.0 & 111.1 \\ C_{14} - C_{16} - C_{20} & 119.6 & 120.0 & C_{42} - C_{47} - H_{48} & 109.0 & 111.2 \\ C_{15} - C_{18} & 120.3 & 120.2 & C_{42} - C_{47} - H_{51} & 109.0 & 111.5 \\ C_{16} - C_{20} - C_{18} & 119.9 & 119.6 & H_{48} - C_{47} - H_{49} & 109.0 & 111.5 \\ C_{16} - C_{20} - C_{18} & 119.9 & 120.2 & H_{48} - C_{47} - H_{49} & 109.0 & 107.4 \\ C_{3} - C_{24} - C_{25} & 119.9 & 120.2 & H_{48} - C_{47} - H_{51} & 109.0 & 107.6 \\ C_{3} - C_{24} - C_{26} & 121.1 & 120.9 & H_{49} - C_{47} - H_{51} & 109.0 & 107.6 \\ C_{25} - C_{24} - C_{26} & 118.8 & 118.8 & Dihedral (^{\circ}) & \\ C_{24} - C_{25} - C_{27} & 120.3 & 120.7 & C_{2} - C_{3} - N_{12} - C_{4} & -66.82 & -62.88 \\ C_{24} - C_{26} - C_{29} & 120.8 & 120.5 & C_{24} - C_{3} - N_{12} - C_{4} & 172.32 & 174.49 \end{array}$	$L_4 - L_{13} - L_{14}$	120.9	120.7	$C_{39} - C_{42} - H_{46}$	109.0	109.2
$\begin{array}{ccccccc} c_{14}-c_{13}-c_{15} & 109.0 & 118.7 & H_{45}-c_{42}-c_{47} & 109.0 & 109.4 \\ c_{13}-c_{14}-C_{16} & 120.9 & 120.8 & H_{46}-C_{42}-C_{47} & 109.0 & 109.4 \\ c_{13}-c_{15}-c_{18} & 120.8 & 120.6 & C_{42}-C_{47}-H_{48} & 109.0 & 111.1 \\ c_{14}-c_{16}-c_{20} & 119.6 & 120.0 & c_{42}-c_{47}-H_{49} & 109.0 & 111.2 \\ c_{15}-c_{18}-c_{20} & 120.3 & 120.2 & C_{42}-c_{47}-H_{51} & 109.0 & 111.5 \\ c_{16}-c_{20}-c_{18} & 119.9 & 119.6 & H_{48}-c_{47}-H_{51} & 109.0 & 107.4 \\ c_{3}-c_{24}-c_{25} & 119.9 & 120.2 & H_{48}-c_{47}-H_{51} & 109.0 & 107.6 \\ c_{3}-c_{24}-c_{26} & 121.1 & 120.9 & H_{49}-c_{47}-H_{51} & 109.0 & 107.6 \\ c_{25}-c_{24}-c_{26} & 118.8 & 118.8 & Dihedral (°) \\ c_{24}-c_{25}-c_{27} & 120.3 & 120.7 & c_{2}-c_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ c_{24}-c_{26}-c_{29} & 120.8 & 120.5 & c_{24}-c_{3}-N_{12}-C_{4} & 172.32 & 174.49 \\ \end{array}$	$L_4 - L_{13} - L_{15}$	120.4	120.5	$H_{45}-C_{42}-H_{46}$	108.0	105.9
$\begin{array}{ccccccc} L_{13}-L_{14}-L_{16} & 120.9 & 120.8 & H_{46}-L_{42}-L_{47} & 109.0 & 109.4 \\ L_{13}-C_{15}-C_{18} & 120.8 & 120.6 & C_{42}-L_{47}-H_{48} & 109.0 & 111.1 \\ C_{14}-C_{16}-C_{20} & 119.6 & 120.0 & C_{42}-C_{47}-H_{49} & 109.0 & 111.2 \\ C_{15}-C_{18}-C_{20} & 120.3 & 120.2 & C_{42}-C_{47}-H_{51} & 109.0 & 111.5 \\ C_{16}-C_{20}-C_{18} & 119.9 & 119.6 & H_{48}-C_{47}-H_{51} & 109.0 & 107.4 \\ C_{3}-C_{24}-C_{25} & 119.9 & 120.2 & H_{48}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{3}-C_{24}-C_{26} & 121.1 & 120.9 & H_{49}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{25}-C_{24}-C_{26} & 118.8 & 118.8 & Dihedral(^\circ) & & \\ C_{24}-C_{25}-C_{27} & 120.3 & 120.7 & C_{2}-C_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ C_{24}-C_{26}-C_{29} & 120.8 & 120.5 & C_{24}-C_{3}-N_{12}-C_{4} & 172.32 & 174.49 \end{array}$	$L_{14} - L_{13} - L_{15}$	109.0	118./	$H_{45}-C_{42}-C_{47}$	109.0	109.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$c_{13} - c_{14} - c_{16}$	120.9	120.8	$H_{46} - C_{42} - C_{47}$	109.0	109.4
$\begin{array}{ccccccc} C_{14}-C_{16}-C_{20} & 119.6 & 120.0 & C_{42}-C_{47}-H_{49} & 109.0 & 111.2 \\ C_{15}-C_{18}-C_{20} & 120.3 & 120.2 & C_{42}-C_{47}-H_{51} & 109.0 & 111.5 \\ C_{16}-C_{20}-C_{18} & 119.9 & 119.6 & H_{48}-C_{47}-H_{49} & 109.0 & 107.4 \\ C_{3}-C_{24}-C_{25} & 119.9 & 120.2 & H_{48}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{3}-C_{24}-C_{26} & 121.1 & 120.9 & H_{49}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{25}-C_{24}-C_{26} & 118.8 & 118.8 & Dihedral (°) \\ C_{24}-C_{25}-C_{27} & 120.3 & 120.7 & C_{2}-C_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ C_{24}-C_{26}-C_{29} & 120.8 & 120.5 & C_{24}-C_{3}-N_{12}-C_{4} & 172.32 & 174.49 \end{array}$	$C_{13} - C_{15} - C_{18}$	120.8	120.6	$C_{42} - C_{47} - H_{48}$	109.0	111.1
$\begin{array}{ccccccc} C_{15}-C_{18}-C_{20} & 120.3 & 120.2 & C_{42}-C_{47}-H_{51} & 109.0 & 111.5 \\ C_{16}-C_{20}-C_{18} & 119.9 & 119.6 & H_{48}-C_{47}-H_{49} & 109.0 & 107.4 \\ C_{3}-C_{24}-C_{25} & 119.9 & 120.2 & H_{48}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{3}-C_{24}-C_{26} & 121.1 & 120.9 & H_{49}-C_{47}-H_{51} & 109.0 & 107.6 \\ C_{25}-C_{24}-C_{26} & 118.8 & 118.8 & Dihedral (°) & & & \\ C_{24}-C_{25}-C_{27} & 120.3 & 120.7 & C_{2}-C_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ C_{24}-C_{26}-C_{29} & 120.8 & 120.5 & C_{24}-C_{3}-N_{12}-C_{4} & 172.32 & 174.49 \end{array}$	$C_{14} - C_{16} - C_{20}$	119.6	120.0	$C_{42} - C_{47} - H_{49}$	109.0	111.2
$\begin{array}{cccccc} C_{16}-C_{20}-C_{18} & 119.9 & 119.6 & H_{48}-C_{47}-H_{49} & 109.0 & 107.4 \\ \hline C_3-C_{24}-C_{25} & 119.9 & 120.2 & H_{48}-C_{47}-H_{51} & 109.0 & 107.6 \\ \hline C_3-C_{24}-C_{26} & 121.1 & 120.9 & H_{49}-C_{47}-H_{51} & 109.0 & 107.6 \\ \hline C_{25}-C_{24}-C_{26} & 118.8 & 118.8 & Dihedral (°) & & & \\ \hline C_{24}-C_{25}-C_{27} & 120.3 & 120.7 & C_{2}-C_{3}-N_{12}-C_{4} & -66.82 & -62.88 \\ \hline C_{24}-C_{26}-C_{29} & 120.8 & 120.5 & C_{24}-C_{3}-N_{12}-C_{4} & 172.32 & 174.49 \end{array}$	$C_{15} - C_{18} - C_{20}$	120.3	120.2	$C_{42} - C_{47} - H_{51}$	109.0	111.5
	$C_{16} - C_{20} - C_{18}$	119.9	119.6	$H_{48} - C_{47} - H_{49}$	109.0	107.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_3 - C_{24} - C_{25}$	119.9	120.2	$H_{48} - C_{47} - H_{51}$	109.0	107.6
$\begin{array}{cccc} C_{25}-C_{24}-C_{26} & 118.8 & 118.8 & Dihedral (^{\circ}) \\ C_{24}-C_{25}-C_{27} & 120.3 & 120.7 & C_2-C_3-N_{12}-C_4 & -66.82 & -62.88 \\ C_{24}-C_{26}-C_{29} & 120.8 & 120.5 & C_{24}-C_3-N_{12}-C_4 & 172.32 & 174.49 \end{array}$	$C_3 - C_{24} - C_{26}$	121.1	120.9	$H_{49}-C_{47}-H_{51}$	109.0	107.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{25} - C_{24} - C_{26}$	118.8	118.8	Dihedral (°)		
C <sub>24</sub> -C <sub>26</sub> -C <sub>29</sub> 120.8 120.5 C <sub>24</sub> -C <sub>3</sub> -N <sub>12</sub> -C <sub>4</sub> 172.32 174.49	$C_{24} - C_{25} - C_{27}$	120.3	120.7	$C_2 - C_3 - N_{12} - C_4$	-66.82	-62.88
	$C_{24} - C_{26} - C_{29}$	120.8	120.5	$C_{24} - C_3 - N_{12} - C_4$	172.32	174.49

Table 1 (Continued)

Parameters Bond length (Å)	Exp.ª	B3LYP/6-31G(d,p)	Parameters Angles Contd.	Exp. <sup>a</sup>	B3LYP/6-31G(d,p)
$C_{25} - C_{27} - C_{31}$	120.8	120.0	$N_{12} - C_4 - C_5 - C_1$	-51.99	-54.54
$C_{26} - C_{29} - C_{31}$	120.7	120.2	$N_{12} - C_4 - C_5 - C_{35}$	-178.04	-179.93
$C_5 - C_{35} - C_{36}$	113.4	113.6	$C_{13} - C_4 - C_5 - C_1$	-172.73	-175.84
$C_{35} - C_{36} - C_{39}$	113.7	112.9	$C_{13} - C_4 - C_5 - C_{35}$	61.21	58.77
$C_{36} - C_{39} - C_{42}$	112.8	113.4	$C_{13} - C_4 - N_{12} - C_3$	-171.28	-172.35
$C_{39} - C_{42} - C_{47}$	113.7	113.2			
$C_2 - C_1 - O_{50}$	121.9	121.8			
$C_2 - C_1 - O_{50}$	122.0	122.9			

<sup>a</sup> Ref. [7].



Fig. 4. Theoretical (a) and experimental (b) FT-Raman spectrum of PDPO.

3317 cm<sup>-1</sup> respectively. The corresponding theoretical frequency for  $\nu_{N-H}$  mode is about 3384 cm<sup>-1</sup>, which shows positive deviation of ~68 cm<sup>-1</sup> from the experimental value. The scissoring mode of N–C–H is appeared at 1407 cm<sup>-1</sup> (FT-IR-strong) and 1409 cm<sup>-1</sup> (FT-Raman-weak), while the harmonic scissoring vibration existed at 1411 cm<sup>-1</sup> (mode no. 104). These  $\delta_{C-N-H}$  wavenumbers are also find support from the literature. Out-of-plane bending modes ( $\gamma_{C-N-H}$ ) are calculated at about 765 and 771 cm<sup>-1</sup> (mode nos. 44, 45), these vibrations are in line with the observed FT-IR (765 cm<sup>-1</sup>) and FT-Raman (785 cm<sup>-1</sup>) bands.

# 4.3.2. Methyl and methylene group vibrations

Methyl groups are generally referred to as electron donating substituents in the aromatic ring system [16]. In acetates, the asymmetric vibrations of the methyl group are expected to occur in the region 2940–3040 cm<sup>-1</sup> and symmetric vibrations are in the region 2910–2930 cm<sup>-1</sup>, and usually the bands are weak [17]. Aromatic acetyl substituents absorb in a narrow range 3000–3020 cm<sup>-1</sup> absorption sometimes coincides with a CH stretching mode of the ring [17]. The title molecule possesses methyl (CH<sub>3</sub>) and methylene (CH<sub>2</sub>) groups. Methyl group symmetric stretching vibrations are appeared at 2914 cm<sup>-1</sup> as a strong intense band in FT-IR and 2913 cm<sup>-1</sup> as a very weak band in FT-Raman spectrum. While the scaled harmonic frequency 2917 cm<sup>-1</sup> (mode no: 127) with considerable intensity is in line with experimental value. The asymmetric of CH<sub>3</sub> harmonic frequency 2987 cm<sup>-1</sup> (mode no: 135) is

coincide well with experimental values (FT-IR: 2989/FT-Raman: 2990 cm<sup>-1</sup>).

The asymmetric and symmetric CH<sub>2</sub> stretching vibrations are normally appear in the region 3100–2900 cm<sup>-1</sup> [18]. According to the literature [18], the observed bands  $2870 \,\mathrm{cm}^{-1}$  (weak), 2924 cm<sup>-1</sup> (strong) in FT-IR and 2890 cm<sup>-1</sup> (weak) FT-Raman are in agreement with the theoretical values in the range of 2891–2937 cm<sup>-1</sup> (mode nos: 123–126, 128–130). The FT-IR band 2956 cm<sup>-1</sup> (strong) and its corresponding theoretical value 2960 cm<sup>-1</sup> (mode no: 132) are attributed  $v_{asy}$  CH<sub>2</sub> vibration. The TED value shows that these vibrations are pure. In aromatic compounds the  $\nu_{C-H}$ ,  $\beta_{C-H}$  and  $\gamma_{C-H}$  modes are appeared in the range of 3000–3100 cm<sup>-1</sup>, 1000–1300 and 750–1000 cm<sup>-1</sup>, respectively [19-21]. The C-H stretching vibrations appeared at 2810, 3048-3077 cm<sup>-1</sup> (mode nos: 122, 137-144). The observed frequencies 2855, 3061  $cm^{-1}$  (FT-IR) and 2856, 3042, 3057  $cm^{-1}$ (FT-Raman) are belongs to C-H stretching mode. The C-H in-plane bending vibrations appeared in the range  $1123-1170 \text{ cm}^{-1}$  (mode nos: 76, 79, 81) and their corresponding experimental wavenumbers 1118, 1145, 1155 (FT-IR) and 1129, 1156 cm<sup>-1</sup> (FT-Raman) are in consistent with computed values. The assignments also find support from the literature [22,23].

The scissoring mode of the CH<sub>2</sub> group gives rise to a characteristic band near  $1415 \text{ cm}^{-1}$  in IR and  $1400 \text{ cm}^{-1}$  in Raman spectra. The twisting, wagging and rocking vibrations appear in the region 1400–900 cm<sup>-1</sup> [24]. The broadening and intensity decreases were observed for the bands at 1470 and 1450 cm<sup>-1</sup> corresponding to CH<sub>2</sub> scissoring modes [22]. In the present investigation,  $\delta_{CH2}$ mode appear at 1436 and 1456 cm<sup>-1</sup> as medium band at FT-IR, and their FT-Raman counter parts are 1452 and 1432 cm<sup>-1</sup> as weak bands. These experimental frequencies are in agreement with mode nos: 106 and 111 of B3LYP. A major coincidence of theoretical values with that of experimental observation is found for  $\omega_{CH2}$ (1348:B3LYP-mode no: 100/1347 cm<sup>-1</sup>: FT-IR). These assignments find support from the literature [22]. In the case of CH<sub>2</sub> twisting mode the vibrational frequencies observed at 1274, 1303 cm<sup>-1</sup> (FT-IR) and 1304 cm<sup>-1</sup> (Raman) are in agreement with the calculated frequencies in the range of 1278–1300 cm<sup>-1</sup> (mode no: 90, 92–94/DFT). The out-of-plane bending mode of C-H always lies in the lower side of spectra. In the present study, the harmonic wavenumbers (mode nos: 60-58, 56, 54-52, 48, 47, 43-40) in the range of 962–706 cm<sup>-1</sup> are assigned to  $\gamma_{C-H}$  mode, which find support from the observed FT-IR frequencies: 912, 889, 757 and  $738 \,\mathrm{cm}^{-1}$ .

# 4.3.3. *C*=*O*, *C*-*N*, *C*=*C* vibrations

Stretching vibration of carbonyl group C=O can be observed as a very strong band in both FT-IR and FT-Raman spectra at 1665 cm<sup>-1</sup> [22]. The carbonyl stretching C=O vibration [17,25] is expected to occur in the region 1715–1680 cm<sup>-1</sup>. The deviation of the calculated wavenumbers for this mode can be attributed to the underestimation of the large degree of  $\pi$ -electron delocalization due to conjugation of the molecule [26]. The literature

Table 2	
Vibrational wave numbers obtained for PDPO at B3LYP/6-31G(d,p).	

Mode no.	Computed va	lues	Experimen	ıtal	Intensity		$\text{TED}^{d} (\geq 10\%)$
	Unscaled	Scaled <sup>a</sup>	FT-IR	FT-Raman	I <sub>IR</sub> <sup>b</sup>	I <sub>Raman</sub> <sup>c</sup>	
1	22	21			0.06	77.4	$\Gamma_{\text{cores}}(40)$
2	27	26			0.09	34.2	$\Gamma_{c25c5c1c2}$ (12), $\Gamma_{c25c5c1050}$ (12)
3	30	29			0.10	68.7	$\Gamma_{c25c24c3N12}$ (16), $\Gamma_{c26c24c3N12}$ (13)
4	40	38			0.04	100	$Γ_{C14C13C4N12}$ (24), $Γ_{C14C13C4C5}$ (21), $Γ_{C15C13C4N12}$ (16)
5	49	47			0.04	2.04	$\Gamma_{\text{CCCC}}$ (20), $\Gamma_{\text{HCCC}}$ (12)
6	49	47			0.00	59.9	$\delta_{\rm NCC}$ (12)
7	77	74			0.71	7.40	$\Gamma_{\rm cccc}$ (13), $\Gamma_{\rm ccco}$ (13)
8	80	77 86			0.01	0.80	$\delta_{CCC}$ (18), I CCCC (10) $\delta_{CCC}$ (19), $\Gamma_{CCCC}$ (15)
10	113	109		109vs	0.10	4 16	$\Gamma_{ccco}(14)$
11	127	122		10010	0.19	2.84	$\Gamma_{c47c42c39c36}(12)$
12	140	135			0.11	1.35	$\Gamma_{\rm CCCC}$ (14)
13	174	167			0.32	7.57	δ <sub>CCC</sub> (26), ν <sub>CC</sub> (16)
14	182	175		184w	0.45	1.05	$\delta_{C26C24C3}(12)$
15	209	201			0.25	6.28	$\delta_{\text{CCC}}$ (15), $\nu_{\text{CC}}$ (14)
16	230	221		215w	0.24	7.64	$\Gamma_{CCCC}(18) \qquad (10) \ \Gamma_{CCCC}(10) \ \Gamma_{CCCC}(10)$
17	250	240		233W	0.00	0.01	$1_{H51C47C42C39}$ (21), $1_{H48C47C42C39}$ (19), $1_{H49C47C42C39}$ (19) $\delta_{recc}$ (24)
19	289	230			0.23	2.54	$\delta_{ccc}(15)$
20	297	285			2.35	2.94	$\delta_{\text{CCC}}(19)$
21	304	292		311w	0.46	2.21	$\delta_{C25C24C3}$ (12), $\delta_{C26C24C3}$ (11)
22	358	344			1.73	1.24	$\nu_{\rm CC}$ (24)
23	378	363			0.16	0.38	$\delta_{C39C36C35}$ (13), $\delta_{C47C42C39}$ (13)
24	417	401			0.09	0.07	$\Gamma_{c20c16c14c13}$ (14), $\Gamma_{c20c18c15c13}$ (13)
25	418	401	426	2.47	0.08	0.19	$1_{C31C27C25C24}$ (14), $1_{C31C29C26C24}$ (13)
20	441	424	456w	547W	1.46	0.66	$\delta_{\text{CCC}}(20)$
27	505	485	400W		6.99	0.00	$\delta_{C2C1050}(10)$
29	524	503	511w		1.61	0.63	$\Gamma_{\rm CCCC}$ (10)
30	541	520	531m	536w	6.46	0.80	$\delta_{\rm NCC}$ (10)
31	573	551	553w		3.67	0.58	δ <sub>CCN</sub> (10)
32	613	589			1.01	0.52	$\delta_{\rm NCC}$ (10)
33	623	599			1.96	2.30	$\delta_{\text{CCC}}(21)$
34	634	609	C12	C10	0.02	2.28	$\delta_{C20C16C14}$ (15), $\delta_{C20C18C15}$ (15)
35	656	630	612W	018111	0.03	3.13	$0_{C31C29C26}(10), 0_{C27C25C24}(14)$
37	676	649		648w	16.1	4.40 5.74	$v_{cc}(10)$ beec (10) $\Gamma_{UNCC}(10)$
38	716	688	661s	665w	15.2	0.73	$\Gamma_{H23C20C16C14}$ (11), $\Gamma_{H23C20C18C15}$ (11)
39	717	689	698s		11.8	0.61	Г <sub>Н34C31C27C25</sub> (10), Г <sub>Н34C31C29C26</sub> (10)
40	734	706			6.29	0.56	Г <sub>НССН</sub> (40)
41	748	719			0.91	0.46	$\nu_{\rm CC}$ (10), $\Gamma_{\rm HCCC}$ (10)
42	775	744	738s		16.6	0.51	$\Gamma_{\text{HCCC}}(26)$
43	781 706	/51 765	757s 765a		7.40	0.57	$\Gamma_{\text{HCCC}}(25)$
44	802	703	703s 784s		6.96	0.51	$\Gamma_{\text{UNCC}}(10)$
46	826	794	7010		1.86	0.33	$\nu_{c13C4}(12)$
47	863	829			0.07	1.06	$\Gamma_{\rm HCCC}$ (46)
48	867	833			0.14	2.23	Γ <sub>HCCC</sub> (58)
49	870	836			0.33	0.42	$\nu_{\rm CC}$ (10)
50	900	864	857w		1.20	2.08	$\nu_{C42C39}$ (25), $\delta_{H51C47C42}$ (17), $\nu_{C47C42}$ (13)
51	917	881	880		0.75	2.04	$\nu_{C3C2}$ (24), $\delta_{N12C3}$ (10), $\delta_{C3C2H}$ (10)
52	920	896	009W		4.56	2.99	$V_{CC}$ (20), I HCCH (10)
55	936	900	912w		1.13	0.61	$\Gamma_{H32(2)/(25H28)}(10)$
55	967	929		919m	0.84	1.30	$\nu_{C3C2}$ (14), $\delta_{CCCH}$ (10)
56	976	938			0.06	0.07	Г <sub>H22C18C15H19</sub> (20), Г <sub>H21C16C14H17</sub> (19)
57	980	941			0.94	0.65	$\nu_{C5C4}$ (14), $\nu_{C36C35}$ (14)
58	980	942			0.51	0.37	Г <sub>H32C27C25H28</sub> (15), Г <sub>H33C29C26H30</sub> (13)
59	1000	961			0.24	0.03	$\Gamma_{H23C20C18H22}$ (23), $\Gamma_{H23C20C16H21}$ (20), $\Gamma_{H22C18C15H19}$ (15)
00 61	1002	962			1.05	0.32	$I_{H34C31C29H33}$ ( $Z_1$ ), $I_{H33C29C26H30}$ ( $I_1$ ), $I_{H34C31C27H32}$ (16)
62	1005	977	973w		0.19	2.52	$\delta_{ccc}(28) \nu_{cc}(16)$
63	1017	977	57544		0.50	12.5	$\delta_{\text{crc}}$ (40)
64	1033	992	986w	988m	0.43	0.64	$\nu_{C47C42}$ (39), $\nu_{C39C36}$ (23)
65	1054	1013	1001w	1003vs	1.74	3.13	$\nu_{C36C35}$ (17), $\nu_{C20C16}$ (12), $\nu_{C20C18}$ (10)
66	1055	1014			4.86	2.07	$\nu_{C31C27}$ (19), $\nu_{C31C29}$ (18)
67	1059	1018	105-		1.18	4.34	$\nu_{\rm C36C35}$ (25)
68	1069	1027	1028w	1030m	0.33	2.71	$\nu_{C42C39}$ (29), $\nu_{C39C36}$ (24), $\nu_{C47C42}$ (21)
09 70	1077	1035	1046.		3.12 2.16	1.23	$\nu_{\rm C35C5}$ (29)
70	1104	1049	1040W		2.10	0.29	$\delta_{CCH}$ (18) $\nu_{CC}$ (9) $\nu_{NC}$ (10)
· •			100000		1.01	0.20	

Table 2 (Continued)

Uncelet         Uncelet         Field $h^{a}$ $h_{con}^{a}$ $h_{con}^{a}$ 73         1130         1066         1067         42.6         2.02 $h_{con}^{a}$ (12), $h_{con}^{a}$ (13), $h_{con}^{a}$ (14), $h_{con}^{a}$ (13), $h_{con}^{a}$ (13), $h_{con}^{a}$ (14), $h_{con}^{a}$ (13), $h_{con}^{a}$ (14), $h_{con}^{a}$ (14), $h_$	Mode no.	Computed value	ues	Experiment	al	Intensity		TED <sup>d</sup> (≥10%)
		Unscaled	Scaled <sup>a</sup>	FT-IR	FT-Raman	I <sub>IR</sub> <sup>b</sup>	I <sub>Raman</sub> c	
11         1130         1086         10860 $426$ 2.22 $erorchologic short (12) erode $	72	1115	1071	1068w		1.77	0.67	ν <sub>N12C4</sub> (11)
74       1144       1009       661       1.31       wc (16) & bcc (17)         75       1169       11189       1129w       402       1.39       Maxeera (17) hore same (17)         77       1187       1141       1149w       0.06       1.32       Maxeera (17) hore same (17)         78       1187       1141       1139w       1.28       Law (18)       Maxeera (17)         79       1204       135       1139w       1.28       Law (12)       Maxeera (17)         81       122       1174	73	1130	1086	1086w		4.26	2.22	$\nu_{C3C2}$ (12), $\nu_{N12C3}$ (12)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	74	1144	1099			6.61	1.31	$\nu_{\rm CC}$ (16), $\delta_{\rm CCC}$ (11), $\nu_{\rm NC}$ (10)
197       1187       1140       118w       102       150       Number of 17.5 Augusts (17)         78       1197       1141       1146w       0.06       1.32       Descript (17) Augusts (16)         79       1264       1156       1135w       1.26       1.46       Server (17) Augusts (16)         80       127       1170       1170       2.08       1.44       Vec (13) Auge (10)         81       1272       1170       1170       2.08       1.44       Vec (13) Auge (10)         84       1242       1193       1173m       1.33       0.62       Vec (13) Auge (10)         85       1246       1197       1200m       1201m       1.35       Kec (13) Vec (10)         86       1244       1224       1224w       1.31       0.65       Kec (14)         90       1333       1261       1223w       1.34       0.66       Kec (14)         91       1335       1283       1.34       0.66       Kec (14)       Kec (14)         91       133       1202       1.30       1.35       Kec (14)       Kec (14)       Kec (14)         91       1333       1283       1324       132       1.35 <t< td=""><td>75 76</td><td>1149</td><td>1104</td><td>1110m</td><td></td><td>5.33</td><td>1.44</td><td><math>\nu_{\rm N12C3}</math> (23) 8 (12) <math>\mu</math> (11)</td></t<>	75 76	1149	1104	1110m		5.33	1.44	$\nu_{\rm N12C3}$ (23) 8 (12) $\mu$ (11)
78       192       1141       1145w       115w       132       1145 $maxsac (17)$ $maxsac (17)$ 80       1275       1158       1158       126       1158 $max (12)$ $max (12)$ 81       1277       1179       1187m       1178m       133       448 $max (12)$ $max (12)$ 83       1227       1179       1187m       1178m       133       448 $max (12)$ $max (12)$ 84       1227       1139       1208m       9.57       4.58 $max (10)$ $max (10)$ 85       1246       1137       1208m       9.57       4.58 $max (10)$ $max (10)$ 86       1238       1247       1241       1227       3.14       0.68 $max (10)$ 90       1330       1273       1274w       2.41       0.68 $max (10)$ 91       1331       128       134       0.68 $max (10)$ $max (10)$ 92       1331       1358       1358       130       130       0.69 $max (10)$ 93       137       1398       1336       130       0.69 $ma$	70	1187	1125	1118w	1129w	4.00	1.35	$\delta_{\text{HCC}}(15), \nu_{\text{NC}}(11)$
79       204       1156       1155w       1125w       1.26       1.45 $h_{crc}(12), h_{crc}(10)$ 81       1217       1170       208       1.46       156       hrc (12), h_{crc}(10)         81       1217       1170       1187m       1187m <td>78</td> <td>1187</td> <td>1141</td> <td>1145w</td> <td>112011</td> <td>0.06</td> <td>1.32</td> <td><math>\delta_{\text{H23C20C16}}(17), \delta_{\text{H23C20C18}}(16)</math></td>	78	1187	1141	1145w	112011	0.06	1.32	$\delta_{\text{H23C20C16}}(17), \delta_{\text{H23C20C18}}(16)$
	79	1204	1156	1155w	1156w	1.26	1.45	δ <sub>CCH</sub> (22), ν <sub>CC</sub> (10)
81       1217       170       20.8       1.46 $u_{c1}(1), 0_{c2}(10)$ 83       1227       113       1137       1137       5.33       6.26 $u_{c1}(2), 0_{c2}(1)$ 84       1242       1133       1137       5.33       6.26 $u_{c1}(2), 0_{c2}(1)$ 85       1246       1197       1200m       1203m       9.57       4.59 $\delta_{cc1}(3)$ $\delta_{cc1}(3)$ 86       1244       1247       1244       1244       0.01       1.15 $\delta_{cc1}(3)$ 87       133       136       1238       1238       1247       1244       0.01       4.66 $\delta_{cc2}(3)$ 98       133       133       1238       1238       1238       0.01       4.76 $\delta_{cc2}(3)$ 94       1333       1308       1308       1308       1308       0.01       0.19 $v_{cc2}(10)$ 95       1361       1378       1338       1328       133       0.01       0.19 $v_{cc2}(10)$ 96       1371       1379       1328       241       0.21       1.15 $\delta_{cc1}(10)$ 97       138       138       1327m	80	1205	1158			0.46	1.56	$\nu_{\rm CC}$ (12)
	81	1217	1170			20.8	1.46	$\nu_{\rm CC}$ (13), $\delta_{\rm HCC}$ (10)
b4       1242       1193       1.00m       1.50m       5.13       0.82 $\lambda_{0cc}(1)$ (Marce (1))         85       1246       1197       120m       1.31       0.65 $\lambda_{0cc}(3)$ , $\nu_{cc}(1)$ 86       1234       1224       1224       1224       0.95       0.30 $\Lambda_{0cc}(20)$ 88       1288       1247       1241       0.91       1.15 $\Lambda_{0cc}(1)$ 0.91         91       133       128       1274       1241       0.99 $\nu_{0cc}(12)$ 0.91         92       1338       1283       128       129       0.14       0.99 $\nu_{0cc}(1)$ 93       1342       128       129       0.51       0.99 $\Lambda_{0cc}(1)$ 94       1333       130m       129       1.01 $\Lambda_{0cc}(1)$ 0.11       0.11	82 83	1222	1174	1187m	1178m	13.5	5.22	$\nu_{C13C4}$ (20)
85       1246       1224       1224       1228       3.62       3.62       13.72       10.05         87       1283       1233       0.05       0.03       5ccc (13)       10.01         88       1313       1281       1233       0.05       5ccr (14)       10.01         88       1313       1281       1231       0.67       1.88       w(14)         91       1335       1283       1284       10.0       4.76       5ccr (12)         92       1338       1283       10.0       4.76       5ccr (13)       6ccr (12)         93       1342       1289       0.10       4.76       5ccr (12)       0.01         94       1353       1306       10.90       wccr (10)       0.01       9ccr (12)       0.01       0.01       9ccr (12)       0.01       0.01       9ccr (12)       0.01       0.01       9ccr (13)       0.01       0.01       0.01       9ccr (12)       0.01       0.02       9ccr (12)       0.01       0.01       9ccr (13)       0.01       0.02       9ccr (13)       0.01       0.02       9ccr (13)       0.01       0.01       0.02       9ccr (13)       0.01       0.01       0.01       9ccr (1	84	1242	1193	1107111	1170111	5.13	0.82	$\delta_{CCH}$ (10), $\delta_{HCC}$ (11)
86         12/4         12/4         1.31         0.65 $\delta_{tot}$ (20)           87         1283         123         0.21         1.15 $\delta_{tot}$ (20)           88         1313         1241         123.02         1.15 $\delta_{tot}$ (10)           91         1333         1281         123.02         1.15 $\delta_{tot}$ (11)           92         1338         1283         1281         1.24         0.05 $\delta_{tot}$ (16)           93         1342         1283         123.0         1.53 $\delta_{tot}$ (17) $\delta_{tot}$ (17)           94         1353         1300         1302         1304m         1.60         0.69 $\delta_{tot}$ (21)           95         1361         1308         1327         1.31         0.60 $\delta_{tot}$ (21) $\delta_{tot}$ (10)           97         1322         1339         1326         1327m         1.26 $\delta_{tot}$ (21)           98         1380         1328         1328m         8.22         1.63 $\delta_{tot}$ (12)           101         144         1388         1327m         1.23 $\delta_{tot}$ (21) $\delta_{tot}$ (21)           102         1447	85	1246	1197	1209m	1203m	9.57	4.59	$\delta_{\text{HCC}}$ (13), $\nu_{\text{CC}}$ (10)
87       128       123       1241       0.55       0.50       bacc (20)         88       139       1297       1241       0.51       1.63       becc (11)         89       139       1297       123       123       becc (12)         91       1335       1283       1284       16.1       1.68       rec (12)         92       138       1283       1284       1.60       0.69       becc (11)         94       1353       1300       1303       1.60       0.69       becc (12)         95       1361       1308       0.91       0.91       vccc6 (10)         96       1361       1308       0.91       0.91       vccc0 (10)         97       1370       130       0.9       becc (12)       vccc0 (13)         100       1403       1348       1347w       2.41       0.21       becc (13)         101       1414       1350       2.41       becc (10)       becc (10)       becc (10)         102       1416       1369       427w       2.02       2.41       becc (10)       becc (10)         103       1427       1371       147w       0.03       becc (10)	86	1274	1224	1222w		1.31	0.65	δ <sub>CCH</sub> (13)
88       128       124       124       124       125       125       125       125       125       125       125       125       125       125       125       125       125       125       125       125       125       125       125       126       127       127       127       127       123       1	87	1283	1233	10.11		0.95	0.30	$\delta_{\rm HCC}(20)$
and bit       1336 1335       1278       241       0.68       try (12) try (12)         91       1335       1283       1278       241       0.68       try (12)         92       1338       1283       1285       213       153       620(13), 620(17)         93       1342       1289       213       153       620(13), 620(17)         94       1351       1306       1303       1304       0.61       0.69       620(13), 620(17)         95       1361       1308       0.91       0.19       Wans(10)         97       1372       1313       1338       1338       1338       8.22       163       620(10)         98       1380       1328       1335       1338       8.22       163       620(12)       60(12)         100       1404       1348       1347       225       0.68       620(13)       660(12)       600(	88	1298	1247	1241W		0.21	1.15	$\delta_{\rm CCH}$ (10)
11       1235       1235       124       0.60 $P_{\rm cristman}^{-1/2}$ 93       1342       1285       10.0       4.76 $P_{\rm cristman}^{-1/2}$ 93       1353       1300       1303       1304m       1.60       0.69 $P_{\rm cristman}^{-1/2}$ 94       1353       1300       1303       1304m       0.51       0.19 $V_{\rm cristman}^{-1/2}$ 95       1361       1308       0.51       0.19 $V_{\rm cristman}^{-1/2}$ $V_{\rm cristman}^{-1/2}$ 97       1372       1319       7.13       1.06 $\Phi_{\rm tristman}^{-1/2}$ $V_{\rm tristman}^{-1/2}$ 98       1380       1326       1324m       1.29 $3.70$ $\Phi_{\rm tristman}^{-1/2}$ $\Phi_{\rm tristman}^{-1/2}$ 100       1403       1348       1347m       2.41       0.21 $\Phi_{\rm tristman}^{-1/2}$	90	1330	1278	1253w 1274w		2.41	0.68	$\nu_{\rm CC}$ (14) $\nu_{\rm CC}$ (14) $\delta_{\rm HCH}$ (11)
93       1342       1285       10.0       4.76 $A_{Car(18)} A_{Car(18)}$ 94       1353       1300       1303       1304       1.60       0.69 $A_{Car(18)} A_{Car(18)}$ 94       1351       1308       0.91       0.19 $A_{Car(18)} A_{Car(18)}$ 96       1361       1308       0.91       0.19 $A_{Car(18)} A_{Car(18)}$ 97       1372       1319       123       129       3.70 $A_{Mac(21)} A_{Car(18)}$ 98       1380       1326       1332m       1238       129       3.70 $A_{Mac(21)} A_{Car(18)}$ 100       1414       1338       1340m       1338m       8.35       1.60 $A_{Car(18)} A_{Car(18)}$ 101       1416       1358       1347       0.57       0.54 $A_{Mac(12)} A_{Car(15)}$ 102       1417       2.20       2.41 $A_{Mac(18)} A_{Car(18)} A_{Car(18)}$ 1.11         105       1475       1417       2.20       2.41 $A_{Mac(18)} A_{Mac(18)} A_{Ma$	91	1335	1283			13.4	0.69	$\nu_{\rm CC}$ (12)
93       1342       129	92	1338	1285			10.0	4.76	$\delta_{C42C39H44}$ (11)
94       133       1300       1304       1.60       0.689       0.6200         95       1361       1308       0.51       0.19       Present (10)         96       1372       1319       0.19       Present (10)         98       1380       1326       1322m       1.29       3.70       5 intract (10)         98       1380       1336       1336m       1322       1.63       Apr:(10)       5 mice (15)         100       1404       1348       1347w       2.85       0.08       Apr:(10)       5 mice (15)         101       1416       130       0.09       0.22       Space (15)       5 mice (15)         103       1467       1407m       1409w       3.50       0.44       Space (15)       Space (15)         105       1475       1411       1407m       1409w       3.50       0.22       Space (12)       Space (13)         106       1493       1434       143em       143em       2.00       2.20       2.41       Space (12)       Space (11)       Space (12)       Space (13)       Space (13)	93	1342	1289			21.3	1.53	$\delta_{\text{CCH}}$ (18), $\delta_{\text{HCC}}$ (17)
33       1361       1368       0.31       0.19       Prains 100         96       1361       1368       1328       1329       7.0       Builder (10)         98       1380       1328       1326m       129       3.70       Builder (10)         99       1380       1338       1347w       2.85       0.08       Scrit (13)         100       1444       1388       2.41       0.21       Builder (12)       Scret (15)         101       1444       1389       2.41       0.20       Builder (12)       Scret (15)         103       1447       177       1972w       0.97       0.44       Sename (12)       Sename (15)         103       1447       177       1972w       0.97       0.44       Sename (12)       Sename (15)         104       1439       1436m       1432w       2.95       0.62       Builder (12)       Sename (11)         105       1449       1436m       1432w       2.95       0.52       Builder (12)       Builder (12) <td< td=""><td>94</td><td>1353</td><td>1300</td><td>1303s</td><td>1304m</td><td>1.60</td><td>0.69</td><td><math>\delta_{C36C35H38}(10)</math></td></td<>	94	1353	1300	1303s	1304m	1.60	0.69	$\delta_{C36C35H38}(10)$
$39$ 132       139       7.13       1.06       Numeric (1) $99$ 1380       1326       1332m       123       7.13       3.70 $\delta_{erg}(13)$ $99$ 187       133       1336m       1338m       8.22       163 $\delta_{erg}(13)$ $100$ 1441       138       2.41       0.21 $\delta_{erg}(10)$ $\delta_{erg}(15)$ $101$ 1444       1380       2.41       0.21 $\delta_{erg}(10)$ $\delta_{erg}(15)$ $102$ 1446       1360       0.49       0.42       wc (10) $\delta_{erg}(15)$ $103$ 1427       1371       132w       0.57       0.54 $\delta_{erg}(16)$ $\delta_{erg}(12)$ $\delta_{erg}(12)$ $106$ 1475       1417       2.00       2.41 $\delta_{erg}(12)$ $\delta_{erg}(12)$ $\delta_{erg}(12)$ $106$ 1443       1439       1432w       2.95       0.68 $\delta_{erg}(13)$ $\delta_{erg}(13)$ $110$ 1544       1455       1456s       1452w       0.70       1.21 $\delta_{erg}(13)$ $\delta_{erg}(12)$ $111$ 1514       1455       1456s       1452w       0.70	95	1361	1308			0.51	0.19	$\nu_{C29C26}$ (10)
98         1380         1326         1337         1338         12.9         3.70         5mm cp (10)           100         1403         1348         1337m         2.85         0.68         5mm cp (13)           101         1414         1358         2.41         0.21         5mm cp (12)           102         1416         1360	97	1372	1319			7.13	1.06	$\delta_{\text{HCC}}(21)$
99         1387         1333         1336m         1338m         8.32         1.63 $\delta_{Crt}(13)$ 100         1403         1348         1347w         2.85         0.08 $\delta_{Crt}(13)$ $\delta_{Crt}(15)$ 101         1414         1358         2.41         0.21 $\delta_{Crt}(13)$ $\delta_{Crt}(15)$ 102         1416         1360         0.49         0.42 $v_{Crt}(15)$ $\delta_{maccrnet}(12)$ $\delta_{maccrnet}(12$	98	1380	1326	1332m		12.9	3.70	$\delta_{\text{H11C3C2}}(10)$
100         143         134         137w         2.85         0.08 $\delta_{Crt}(10), \delta_{IRC}(15)$ 101         1414         1358         2.41         0.21 $\delta_{IRC}(12), \delta_{IRC}(15)$ 102         1416         1360         0.49         0.42         Vc. (10), $\delta_{IRC}(12), \delta_{CRC}(15), \delta_{IRSCPARD}(15)$ 104         1468         1411         1407m         1409w         30.5         0.94 $\delta_{CRLTBR}(21), \delta_{CRLTBR}(21), \delta_{IRSCPARD}(15)$ 106         1433         1434         1436m         1432w         2.95         0.68 $\delta_{RTCSBRR}(23)$ 107         1489         1439         -         4.66         0.33 $\delta_{IRCCBRR}(23)$ 108         1500         1442         0.27         1.02 $\delta_{IRCCBRR}(13)$ 111         1514         1458         1452w         2.70         2.91 $\delta_{IRCCBRR}(13)$ 112         1517         1488         1447w         .58         0.30         Vrc (23)           113         1527         1467         .58         0.30         Vrc (23)           114         1538         1477         .58         0.30         Vrc (23)	99	1387	1333	1336m	1338m	8.32	1.63	δ <sub>CCH</sub> (13)
101       1414       138       2.41       0.21       bresk (12)       bresk (12)         102       1416       1360       0.49       0.42       Preck (10), bick (12), bick (15), bisker/met (15)         103       1427       1371       1372w       0.57       0.54       bisker/met (12), bisker/met (15)         105       1475       1417       2.20       2.41       bisker/met (12), bisker/met (15)         106       1493       1434       135m       1432       2.95       0.68       bisker/met (28)         107       1497       1439       7.59       0.22       bisker/met (12), bisker/met (11)         108       1442       0.08       5.92       bisker/met (13)       bisker/met (13)         110       1504       1445       1.456s       1.452w       2.70       2.91       bisker/met (13)         111       1514       1455       1.456s       1.452w       2.70       2.91       bisker/met (13)         1114       1538       1477       7.05       0.03       Verc (23)       1.01         113       1527       1467       1.58       0.19       bisker/met (2)       1.01         114       1538       1478       1493m       <	100	1403	1348	1347w		2.85	0.08	$δ_{\rm CCH}$ (10), $δ_{\rm HCC}$ (15)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	101	1414	1358			2.41	0.21	$\delta_{\text{HCN}}(12)$
	102	1416	1360	1372w/		0.49	0.42	$V_{CC}$ (10), $O_{HCC}$ (12), $O_{CCC}$ (15)
106         1475         1417         2.20         2.41         Spacera (28)           106         1493         1436m         1432w         2.95         0.68         Spacera (28)           107         1497         1439         7.59         0.22         Spacera (23)           108         1498         1439         4.66         0.33         Spacera (28)           109         1500         1442         0.27         1.02         Spacera (19)           110         1504         1445         0.27         1.02         Spacera (28)         Spacera (28)           111         1514         1455         1456s         1452w         2.70         2.91         Spacera (28)         Spacera (28)           112         1517         1487         1493m         0.10         1.13         Spacera (28)         Spacera (28)           113         1527         1467         7.55         0.03         WC (23)           114         1538         1478         1493m         4.46         7.59         WC (20)           114         1538         1478         1493m         4.89         5.28         WC (23)           116         1661         1596         1601w<	105	1468	1411	1407m	1409w	30.5	0.94	$\delta_{C3N12H8}$ (21), $\delta_{C4N12H8}$ (21)
106         1493         1434         1436m         1432w         2.95         0.68         5paccores (12)         matrix           107         1497         1439	105	1475	1417			2.20	2.41	$\delta_{\rm H6C2H7}$ (28)
107       1497       1439       7.59       0.22 $\mathfrak{b}_{1343(127)}(21), \mathfrak{b}_{1343(125)}(11), \mathfrak{b}_{1343(125)}(12), $	106	1493	1434	1436m	1432w	2.95	0.68	δ <sub>H37C35H38</sub> (23)
108       1498       1439       4.6b       0.33       0122CRC16 (11), 0122CRC16 (11), 0122CRC16 (10)         109       1500       1442       0.27       1.02 $b_{145CCR16}$ (13)         111       1514       1455       1456s       1452w       2.70       2.91 $b_{145CCR16}$ (13), $b_{145CCR16}$ (12)         112       1517       1458       0.10       1.13 $b_{145CCR16}$ (13), $b_{145CCR16}$ (11)         113       1527       1467       7.05       0.03 $vcc (23)$ 114       1538       1477       7.05       0.03 $vcc (23)$ 116       1641       1576       1559w       0.15       0.75 $vcacts (10), vcacts (11)$ 117       1642       1577       1585w       1586m       1.09       1.24 $vcacts (20), vcacts (20)$ 119       1662       1597       1654w       1604s       2.46       7.59 $vcacts (20), vcacts (20)         120       1803       1732       1715xbs       1714m       100       1.41       vgass (20), vcacts (20)         121       2923       2809       2808m       6.00       0.17       vcatts (30), vcatts (30)         122       3025       $	107	1497	1439			7.59	0.22	$\delta_{\text{H34C31C27}}$ (12), $\delta_{\text{H34C31C29}}$ (11)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	108	1498	1439			4.66	0.33	$\delta_{H23C20C16}$ (11), $\delta_{H23C20C18}$ (10)
111       1514       1455       1456s       1452w       2.70       2.91       Shaaccrist (28), Shaccrist (23)         112       1517       1488       0.10       1.13       Shaaccrist (15), Shaccrist (11)         114       1538       1477       7.05       0.03       Vcc (23)         115       1538       1478       1493m       4.49       0.03       Vcc (23)         116       1641       1576       1559w       0.15       0.75       Vc2016 (13), Vc20218 (11)         117       1642       1577       1586m       1.09       1.24       Vc3017 (20), Vc30218 (10)         118       1661       1596       1601w       1.89       5.28       Vc3014 (20), Vc30216 (20)         120       1803       1732       1715w       1714m       100       1.41       Vc3044 (38), Vc3044 (10)         121       2923       2809       280m       6.00       0.17       Vc409 (71), Vc3011 (29)         122       2925       2810       285s       2856m       40.8       3.01       Vc3044 (40), Vc2048 (40), Vc3048 (4	110	1504	1442			0.08	1.02	$\delta_{\mu_{45}}$
112       1517       1458	111	1514	1455	1456s	1452w	2.70	2.91	$\delta_{\rm H48C47H51}$ (28), $\delta_{\rm H49C47H51}$ (23)
113       1527       1467       1.58       0.19 $\delta_{\text{HacCrins}}(11)$ 114       1538       1477       7.05       0.03 $\nu_{CC}(23)$ 115       1538       1478       1493m       4.49       0.30 $\nu_{CC}(23)$ 116       1641       1576       1559w       0.15       0.75 $\nu_{Cacts}(13), \nu_{Cacts}(10), \dots_{C31C2}(11)$ 117       1642       1577       1585w       1586m       1.09       1.24 $\nu_{C372}(23), \nu_{C32C3}(20), \nu_{C32C6}(20)$ 119       1662       1597       1654w       1604s       2.46       7.59 $\nu_{C37C3}(20), \nu_{C32C6}(20)$ 121       2923       2809       2808m       6.00       0.17 $\nu_{CHH}(71), \nu_{CHH}(29)$ 122       2925       2810       2855x       2856m       40.8       3.01 $\nu_{CHH}(71), \nu_{CHH}(29)$ 124       3014       2890       3.21       2.85 $\nu_{CHH}(71), \nu_{CHH}(29)$ 121         125       3024       2905       13.3       0.88 $\nu_{CHH}(71), \nu_{CHH}(24), \nu_{CHH}(10)$ 126       3025       2907       15.2       2.36 $\nu_{CHH}(71), \nu_{CHH}(24), \nu_{CHH}(10)$ 127	112	1517	1458			0.10	1.13	$δ_{H48C47H49}$ (15), $δ_{H40C36H41}$ (11)
114       1538       1477       7.05       0.03 $\nu_{CC}(23)$ 115       1538       1478       1493m       4.49       0.30 $\nu_{CC}(23)$ 116       1641       1576       1559w       0.15       0.75 $\nu_{C20C16}(13), \nu_{C20C18}(11)$ 117       1642       1577       1585w       1586m       1.09       1.24 $\nu_{C1C12}(20), \nu_{C1S15}(20)$ 118       1661       1596       1601w       1.89       5.28 $\nu_{C1C12}(20), \nu_{C1S15}(20)$ 120       1803       1732       1715vs       1714m       100       1.41 $\nu_{060C1}(90)$ 121       2923       2809       2808m       6.00       0.17 $\nu_{C4H1}(71), \nu_{C4H1}(29)$ 123       3004       2896       3.82       0.34 $\nu_{C3H44}(40), \nu_{C2H45}(24), \nu_{C3H1}(21)$ 124       3014       2896       3.82       0.34 $\nu_{C3H44}(70)$ 125       3024       2907       15.2       2.36 $\nu_{C3H64}(44), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(24), \nu_{C3H44}(25)         126       3025       2907       5.29       1.45       \nu_{C3H6}(82), \nu_{C3H4}(83), \nu_{C3H44}(2$	113	1527	1467			1.58	0.19	$\delta_{\rm H48C47H49}(11)$
115       1536       1476       149311       4.49       0.30       PCC (23)         116       1641       1576       1559w       0.15       0.75       PConcis (13), PConcis (11), PC31(29) (11)         117       1642       1577       1585w       1586m       1.09       1.24       PC1027 (13), PConcis (20), PC35(28) (20)         119       1661       1596       1601w       1.89       5.28       PC102(2), PC35(2) (20)       C23(2)         120       1803       1732       1715vs       1714m       100       1.41       P050(10), PC311(29)         121       2923       2809       2808m       6.00       0.17       PC314(46), PC314(10)         124       3014       2896       3.82       0.34       PC3644(4), PC314(10)         124       3014       2896       3.82       0.34       PC3644(4), PC314(2), PC314(10)         125       3024       2905       13.3       0.88       PC3144(42), PC3146(2), PC314(2), PC314(2)         126       3025       2907       15.2       2.36       PC3146(37), PC3148(33), PC314(26)         128       3039       2920       2924s       3.68       2.61       PC31446(42), PC3147(42), PC3145(23)         130       3	114	1538	1477	1402		7.05	0.03	$\nu_{\rm CC}$ (23)
117       1641       1577       1585w       1586m       1.0       0.13       PLANE NET (13), PLANE (10),	115	1538	1478	1493111 1559w/		4.49	0.30	$V_{CC}(23)$
118       1661       1596       1601w       1.89       5.28       VCIGCI 4 (20), VCIBCI 5 (20)         119       1662       1597       1654w       1604s       2.46       7.59       VCITCGI 4 (20), VCIBCI 5 (20)         120       1803       1732       1715v       1714m       100       1.41       Voising 7 (20), VCIBCI 5 (20)         121       2923       2809       2808m       6.00       0.17       VCHII (71), VCHII (29)         122       2925       2810       2855s       2856m       40.8       3.01       VCHII (71), VCHII (29)         123       3009       2891       2870w       2890w       3.21       2.85       PC3HAI (46), VCHIA (28), VCHII (10)         124       3014       2896	117	1642	1577	1585w	1586m	1.09	1.24	$\nu_{C31C27}$ (13), $\nu_{C26C24}$ (10), $\nu_{C31C29}$ (11)
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	118	1661	1596	1601w		1.89	5.28	$\nu_{C16C14}$ (20), $\nu_{C18C15}$ (20)
120       1803       1732       171 5vs       171 4m       100       1.41       νoscc1 (90)         121       2923       2809       2808m       6.00       0.17       νC4H9 (71), νC4H1 (29)         122       2925       2810       2850s       2856m       40.8       3.01       vC3H41 (71), vC4H9 (29)         123       3009       2891       2870w       2890w       3.21       2.85       VC3H44 (38), vC3H44 (38), vC3H41 (10)         124       3014       2896       3.82       0.34       vC3H46 (44), vC2H45 (24), vC3H4 (21)         125       3024       2907       15.2       2.36       vC3H46 (37), vC4H44 (33), vC3H44 (22), vC3H45 (24), vC3H1 (26)         126       3025       2907       15.2       2.36       vC3H46 (37), vC4H44 (33), vC4H45 (26)         128       3039       2920       2924s       3.68       2.61       vC3H44 (21), vC3H44 (31), vC4H45 (26)         129       3049       2929       162       1.72       vC3H44 (21), vC3H44 (25), vC3H4 (26)         130       3057       2937       5.29       1.45       vC2H6 (82), vC2H7 (16)         131       3061       2940       2949w       1.75       2.04       vC3H44 (45), vC3H44 (26), vC3H47 (20)	119	1662	1597	1654w	1604s	2.46	7.59	$\nu_{C27C25}$ (20), $\nu_{C29C26}$ (20)
121292328092808m6.000.17PCdB (71, VCBH1 (29)1222925281028552856m40.83.01VCBH1 (71), VCBH1 (29)123300928912870w2890w3.212.85VC39H4 (46), VC39H4 (38), VC36H4 (10)124301428963.820.34VC36H4 (70)1253024290515.22.36VC41H6 (24), VC2H45 (24), VC3H10 (21)1263025290715.22.36VC41H6 (37), VC47H8 (33), VC47H51 (26)127303629172914s2913w19.53.90VC47H49 (37), VC47H8 (33), VC47H51 (26)128303929202924s3.682.61VC3H14 (42), VC3H14 (10)130305729375.291.45VC2H6 (82), VC3H7 (16)1313061294114.90.24VC4BH49 (32), VC2H6 (26), VC3H44 (15)133310129799.650.06VC3BH38 (23), VC3 H17 (20)133310129799.650.06VC3BH38 (23), VC3 H17 (20)1343105298344.30.89VC4H49 (3), VC4H8 (17), VC4H49 (10)136313531022029m6.522.04VC2H17 (83), VC4H8 (17), VC4H49 (10)137317230483042w3.110.76VC2BH28 (68), VC2H32 (22)138317430492.880.62VC1H17 (63), VC4H8 (17), VC4H49 (10), VC2H43 (16), VC2H42 (17)14031813057305750.132.88VC1	120	1803	1732	1715vs	1714m	100	1.41	$\nu_{050C1}(90)$ (20)
122       2053       2010       2053       2050       2050       100       100         123       3009       2891       2870w       2890w       3.21       2.85       PC3H3 (46), VC3H4 (38), VC36H41 (10)         124       3014       2896       3.82       0.34       VC36H41 (70)         125       3024       2905       13.3       0.88       VC2H46 (44), VC3H4 (24), VC3H10 (21)         126       3025       2907       15.2       2.36       VC3H10 (72), VC4H4 (33), VC4H51 (26)         127       3036       2917       2914s       2913w       19.5       3.90       VC4H46 (42), VC3H43 (33), VC4H51 (26)         128       3039       2920       2924s       3.68       2.61       VC3H43 (32), VC4H51 (22)         129       3049       2929       16.2       1.72       VC3H43 (32), VC4H45 (23), VC4H44 (15)         130       3057       2937       5.29       1.45       VC2H46 (20), VC2H45 (22), VC2H4 (26), VC3H44 (15)         132       3081       2960       2956s       1.75       2.04       VC3H43 (32), VC2H46 (21), VC3H44 (31), VC3 H37 (20)         133       3101       2979       9.65       0.06       VC3H48 (32), VC2H46 (20), VC3H48 (31), VC3 H37 (20)         133<	121	2923	2809	2808111	2856m	40.8	0.17	$V_{C4H9}(71), V_{C3H11}(29)$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	122	3009	2891	28503 2870w	2890w	3.21	2.85	$\nu_{C39H43}$ (46), $\nu_{C39H44}$ (38), $\nu_{C36H41}$ (10)
125       3024       2905       13.3       0.88 $\nu_{42H46}$ (44), $\nu_{62H45}$ (24), $\nu_{C5H10}$ (21)         126       3025       2907       15.2       2.36 $\nu_{C5H10}$ (72), $\nu_{62H46}$ (10)         127       3036       2917       2914s       2913w       19.5       3.90 $\nu_{C4H49}$ (37), $\nu_{C4H48}$ (33), $\nu_{C4H51}$ (26)         128       3039       2920       2924s       3.68       2.61 $\nu_{C3H49}$ (42), $\nu_{C3H43}$ (19), $\nu_{C42H45}$ (23)         129       3049       2929       16.2       1.72 $\nu_{C3H45}$ (22), $\nu_{C2H7}$ (16)         130       3057       2937       5.29       1.45 $\nu_{C42H45}$ (32), $\nu_{C3H44}$ (23), $\nu_{C3H44}$ (15)         132       3081       2960       2956s       1.75       2.04 $\nu_{C42H45}$ (32), $\nu_{C3H44}$ (38), $\nu_{C3H44}$ (15)         133       3101       2979       9.65       0.06 $\nu_{C3H44}$ (43), $\nu_{C4H44}$ (43), $\nu_{C4H44}$ (43), $\nu_{C3H44}$ (43), $\nu_{C3H44}$ (43), $\nu_{C3H44}$ (43), $\nu_{C3H44}$ (43) $\nu_{C4H46}$ (44), $\nu_{C4H46}$ (44), $\nu_{C4H46}$ (44) $\nu_{C4H46}$ (44), $\nu_{C4H46}$ (44) $\nu_{C4H46}$ (44) $\nu_{C3H44}$ (43) $\nu_{C4H46}$ (44), $\nu_{C4H46}$ (43) $\nu_{C3H44}$ (43), $\nu_{C3H44}$ (43) $\nu_{C3H44}$ (43) $\nu_{C3H44}$ (43) $\nu_{C3H44}$ (43) $\nu_{C3H44}$ (43) $\nu_{C3H44}$ (4	124	3014	2896			3.82	0.34	$\nu_{\rm C36H41}$ (70)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	125	3024	2905			13.3	0.88	$\nu_{C42H46}$ (44), $\nu_{C42H45}$ (24), $\nu_{C5H10}$ (21)
127303629172914s2913w19.53.90 $\nu_{C47H49}$ (37), $\nu_{C47H48}$ (33), $\nu_{C47H48}$ (26)128303929202924s3.682.61 $\nu_{C39H44}$ (42), $\nu_{C39H3}$ (51), $\nu_{C39H3}$ (51), $\nu_{C39H3}$ (51), $\nu_{C39H3}$ (51), $\nu_{C39H3}$ (51), $\nu_{C39H3}$ (51), $\nu_{C39H44}$ (23)130305729375.291.45 $\nu_{C39H44}$ (26), $\nu_{C39H4}$ (15)1313061294114.90.24 $\nu_{C42H45}$ (32), $\nu_{C42H46}$ (26), $\nu_{C39H44}$ (15)132308129602956s1.752.04 $\nu_{C36H40}$ (46) $\nu_{C35H38}$ (23), $\nu_{C35 H37}$ (20)133310129799.650.06 $\nu_{C35H38}$ (32), $\nu_{C3H40}$ (11), $\nu_{C35 H37}$ (20)1343105298344.30.89 $\nu_{C47H48}$ (43), $\nu_{C47H48}$ (17), $\nu_{C3H44}$ (10)136313530123029m6.522.04 $\nu_{C2H7}$ (83), $\nu_{C2H46}$ (17)137317230483042w3.110.76 $\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)138317430492.880.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)139318130560.182.37 $\nu_{C29H33}$ (46), $\nu_{C3H44}$ (15), $\nu_{C25H28}$ (17)140318130573057s0.132.88 $\nu_{C13H22}$ (37), $\nu_{C29H33}$ (28), $\nu_{C14H17}$ (19)1433202307720.41.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (28), $\nu_{C14H17}$ (13)	126	3025	2907	2014	2012	15.2	2.36	$\nu_{\rm C5H10}$ (72), $\nu_{\rm C42H46}$ (10)
12930392920292453.062.01 $\nu_{C39H4}$ (42), $\nu_{C3H3}$ (13), $\nu_{C32H3}$ (23)1293049292916.21.72 $\nu_{C39H4}$ (42), $\nu_{C3H7}$ (16)130305729375.291.45 $\nu_{C3H46}$ (26), $\nu_{C3H44}$ (15)1313061294114.90.24 $\nu_{C42H45}$ (32), $\nu_{C42H46}$ (26), $\nu_{C39H44}$ (15)132308129602956s1.752.04 $\nu_{C36H40}$ (46) $\nu_{C35H38}$ (23), $\nu_{C35}$ H37 (20)133310129799.650.06 $\nu_{C35H38}$ (32), $\nu_{C36H40}$ (11), $\nu_{C35}$ H37 (20)1343105298344.30.89 $\nu_{C47H48}$ (17), $\nu_{C3H48}$ (17)135310929872989w2990w22.93.03 $\nu_{C47H51}$ (72), $\nu_{C47H48}$ (17), $\nu_{C47H49}$ (10)136313530123029m6.522.04 $\nu_{C2H7}$ (83), $\nu_{C2H6}$ (17)137317230483042w3.110.76 $\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)138317430492.880.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)139318130560.182.37 $\nu_{C29H33}$ (46), $\nu_{C3H34}$ (31), $\nu_{C25H28}$ (17)140318130573057s0.132.88 $\nu_{C18H22}$ (47), $\nu_{C29H33}$ (28), $\nu_{C14H17}$ (19)1413192306713.62.21 $\nu_{C16H21}$ (35), $\nu_{C16H21}$ (23), $\nu_{C20H23}$ (28), $\nu_{C14H17}$ (13)1433202307720.41.22 $\nu_{C15H19}$ (3), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23) <td>127</td> <td>3036</td> <td>2917</td> <td>2914s</td> <td>2913w</td> <td>19.5</td> <td>3.90</td> <td><math>\nu_{C47H49}(37), \nu_{C47H48}(33), \nu_{C47H51}(26)</math></td>	127	3036	2917	2914s	2913w	19.5	3.90	$\nu_{C47H49}(37), \nu_{C47H48}(33), \nu_{C47H51}(26)$
130305729375.291.45 $\nu_{C2H6}(82), \nu_{C2H7}(16)$ 1313061294114.90.24 $\nu_{C42H45}(32), \nu_{C2H7}(16)$ 132308129602956s1.752.04 $\nu_{C36H40}(46) \nu_{C35H38}(23), \nu_{C35 H37}(20)$ 133310129799.650.06 $\nu_{C35H38}(32), \nu_{C36H40}(31), \nu_{C35 H37}(20)$ 1343105298344.30.89 $\nu_{C47H48}(43), \nu_{C47H48}(17), \nu_{C47H48}(17)$ 135310929872989w2990w22.93.03 $\nu_{C47H41}(17), \nu_{C47H48}(17), \nu_{C47H49}(10)$ 136313530123029m6.522.04 $\nu_{C2H7}(83), \nu_{C2H6}(17)$ 137317230483042w3.110.76 $\nu_{C25H28}(68), \nu_{C2TH2}(22)$ 138317430492.880.62 $\nu_{C1H117}(62), \nu_{C16H21}(24)$ 139318130560.182.37 $\nu_{C29H33}(46), \nu_{C3H34}(31), \nu_{C25H28}(17)$ 140318130573057s0.132.88 $\nu_{C1H22}(27), \nu_{C2H32}(23), \nu_{C2H43}(26), \nu_{C14H17}(19)$ 141319130663061m9.093.01 $\nu_{C2H32}(37), \nu_{C29H33}(28), \nu_{C3H34}(15), \nu_{C25H28}(11)$ 1433202307720.41.22 $\nu_{C15H19}(33), \nu_{C16H21}(25), \nu_{C20H23}(28)$	128	3049	2920	25245		16.2	1 72	$\nu_{\rm C39H44}$ (42), $\nu_{\rm C39H43}$ (15), $\nu_{\rm C42H45}$ (23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	130	3057	2937			5.29	1.45	$\nu_{\rm C2H6}$ (82), $\nu_{\rm C2H7}$ (16)
132       3081       2960       2956s       1.75       2.04 $\nu_{C36H40}$ (46) $\nu_{C35H38}$ (23), $\nu_{C35 H37}$ (20)         133       3101       2979       9.65       0.06 $\nu_{C35H38}$ (32), $\nu_{C35 H37}$ (20)         134       3105       2983       44.3       0.89 $\nu_{C47H49}$ (43), $\nu_{C37H49}$ (17), $\nu_{C47H48}$ (17), $\nu_{C47H48}$ (17)         136       3135       3012       3029m       6.52       2.04 $\nu_{C47H47}$ (83), $\nu_{C27H48}$ (17), $\nu_{C47H49}$ (10)         137       3172       3048       3042w       3.11       0.76 $\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)         138       3174       3049       2.88       0.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)         139       3181       3056       0.18       2.37 $\nu_{C29H33}$ (46), $\nu_{C31H34}$ (31), $\nu_{C25H28}$ (17)         140       3181       3057       3057s       0.13       2.88 $\nu_{C14H17}$ (62), $\nu_{C14H17}$ (19)         141       3191       3066       3061m       9.09       3.01 $\nu_{C27H32}$ (37), $\nu_{C29H33}$ (28), $\nu_{C14H17}$ (19)         142       3192       3067       13.6       2.21 $\nu_{C16H21}$ (35), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (28), $\nu_{C20H23}$ (18), $\nu_{C14H17}$ (13)         143       3202 <td< td=""><td>131</td><td>3061</td><td>2941</td><td></td><td></td><td>14.9</td><td>0.24</td><td><math>\nu_{C42H45}</math> (32), <math>\nu_{C42H46}</math> (26), <math>\nu_{C39H44}</math> (15)</td></td<>	131	3061	2941			14.9	0.24	$\nu_{C42H45}$ (32), $\nu_{C42H46}$ (26), $\nu_{C39H44}$ (15)
133       3101       29/9       9.65       0.06 $\nu_{C35H38}$ (32), $\nu_{C36H40}$ (31), $\nu_{C35 H37}$ (20)         134       3105       2983       44.3       0.89 $\nu_{C47H49}$ (43), $\nu_{C47H48}$ (38)         135       3109       2987       2989w       2990w       22.9       3.03 $\nu_{C47H49}$ (43), $\nu_{C47H48}$ (17), $\nu_{C47H49}$ (10)         136       3135       3012       3029m       6.52       2.04 $\nu_{C217}$ (83), $\nu_{C2H6}$ (17)         137       3172       3048       3042w       3.11       0.76 $\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)         138       3174       3049       2.88       0.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)         139       3181       3056       0.18       2.37 $\nu_{C29H33}$ (46), $\nu_{C3H134}$ (31), $\nu_{C25H28}$ (17)         140       3181       3057       3057s       0.13       2.88 $\nu_{C18H22}$ (47), $\nu_{C20H23}$ (26), $\nu_{C14H17}$ (19)         141       3191       3066       3061m       9.09       3.01 $\nu_{C27H32}$ (37), $\nu_{C29H33}$ (28), $\nu_{C14H17}$ (13)         142       3192       3067       13.6       2.21 $\nu_{C16H21}$ (35), $\nu_{C16H21}$ (25), $\nu_{C10H23}$ (23), $\nu_{C14H17}$ (13)         143       3202       3077	132	3081	2960	2956s		1.75	2.04	$\nu_{C36H40}$ (46) $\nu_{C35H38}$ (23), $\nu_{C35}$ H37 (20)
134       3105       2953       44.3       0.89 $\nu_{C47H49}$ (43), $\nu_{C47H48}$ (38)         135       3109       2987       2989w       2990w       22.9       3.03 $\nu_{C47H49}$ (17), $\nu_{C47H48}$ (17), $\nu_{C47H49}$ (10)         136       3135       3012       3029m       6.52       2.04 $\nu_{C27F(83)}$ , $\nu_{C2H6}$ (17)         137       3172       3048       3042w       3.11       0.76 $\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)         138       3174       3049       2.88       0.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)         139       3181       3056       0.18       2.37 $\nu_{C29H33}$ (46), $\nu_{C3H134}$ (31), $\nu_{C25H28}$ (17)         140       3181       3057       3057s       0.13       2.88 $\nu_{C18H22}$ (47), $\nu_{C20H23}$ (26), $\nu_{C14H17}$ (19)         141       3191       3066       3061m       9.09       3.01 $\nu_{C27H32}$ (37), $\nu_{C29H33}$ (28), $\nu_{C14H17}$ (19)         142       3192       3067       13.6       2.21 $\nu_{C16H21}$ (35), $\nu_{C16H21}$ (25), $\nu_{C10H23}$ (23), $\nu_{C14H17}$ (13)         143       3202       3077       20.4       1.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)	133	3101	2979			9.65	0.06	$\nu_{C35H38}$ (32), $\nu_{C36H40}$ (31), $\nu_{C35 H37}$ (20)
136       3135       3012       3029m       6.52       2.04 $\nu_{C2H7}(83), \nu_{C2H4}(17), \nu_{C4H48}(17), \nu_{C4H$	134	3109	2987	2989w	2990w	44.5 22.9	3.03	$\nu_{C47H49}$ (4), $\nu_{C47H48}$ (30) $\nu_{C47H51}$ (72) $\nu_{C47H48}$ (17) $\nu_{C47H49}$ (10)
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	136	3135	3012	3029m	2000	6.52	2.04	$\nu_{C2H7}$ (83), $\nu_{C2H6}$ (17)
138       3174       3049       2.88       0.62 $\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)         139       3181       3056       0.18       2.37 $\nu_{C29H33}$ (46), $\nu_{C31H34}$ (31), $\nu_{C25H28}$ (17)         140       3181       3057       3057s       0.13       2.88 $\nu_{C18H22}$ (47), $\nu_{C20H23}$ (26), $\nu_{C14H17}$ (19)         141       3191       3066       3061m       9.09       3.01 $\nu_{C27H32}$ (37), $\nu_{C29H33}$ (28), $\nu_{C31H34}$ (15), $\nu_{C25H28}$ (11)         142       3192       3067       13.6       2.21 $\nu_{C16H21}$ (35), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (18), $\nu_{C14H17}$ (13)         143       3202       3077       20.4       1.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)	137	3172	3048		3042w	3.11	0.76	$\nu_{C25H28}$ (68), $\nu_{C27H32}$ (22)
139       3181       3056       0.18       2.37 $\nu_{C29H33}$ (46), $\nu_{C31H34}$ (31), $\nu_{C25H28}$ (17)         140       3181       3057       3057s       0.13       2.88 $\nu_{C18H22}$ (47), $\nu_{C20H23}$ (26), $\nu_{C14H17}$ (19)         141       3191       3066       3061m       9.09       3.01 $\nu_{C27H32}$ (37), $\nu_{C29H33}$ (28), $\nu_{C31H34}$ (15), $\nu_{C25H28}$ (11)         142       3192       3067       13.6       2.21 $\nu_{C16H21}$ (35), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (18), $\nu_{C14H17}$ (13)         143       3202       3077       20.4       1.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)	138	3174	3049			2.88	0.62	$\nu_{C14H17}$ (62), $\nu_{C16H21}$ (24)
140318130573057s0.132.88 $v_{C18H22}$ (47), $v_{C20H23}$ (26), $v_{C14H17}$ (19)141319130663061m9.093.01 $v_{C27H32}$ (37), $v_{C29H33}$ (28), $v_{C31H34}$ (15), $v_{C25H28}$ (11)1423192306713.62.21 $v_{C16H21}$ (35), $v_{C18H22}$ (23), $v_{C20H23}$ (18), $v_{C14H17}$ (13)1433202307720.41.22 $v_{C15H19}$ (33), $v_{C16H21}$ (25), $v_{C20H23}$ (23)	139	3181	3056		2057	0.18	2.37	$\nu_{C29H33}$ (46), $\nu_{C31H34}$ (31), $\nu_{C25H28}$ (17)
14151515000500111 $5.05$ $5.01$ $\nu_{C27H32}$ (57), $\nu_{C29H33}$ (20), $\nu_{C31H34}$ (15), $\nu_{C25H28}$ (11)1423192306713.62.21 $\nu_{C16H21}$ (35), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (18), $\nu_{C14H17}$ (13)1433202307720.41.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)	140 141	3181 3101	3057 3066	3061m	3U57S	0.13	2.88	$\nu_{c18H22}$ (47), $\nu_{c20H23}$ (26), $\nu_{c14H17}$ (19)
143       3202       3077       20.4       1.22 $\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)	142	3192	3067	500111		13.6	2.21	$\nu_{C2/H32}$ (37), $\nu_{C29H33}$ (26), $\nu_{C31H34}$ (13), $\nu_{C25H28}$ (11) $\nu_{C16H21}$ (35), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (18). $\nu_{C14H17}$ (13)
	143	3202	3077			20.4	1.22	$\nu_{C15H19}$ (33), $\nu_{C16H21}$ (25), $\nu_{C20H23}$ (23)

#### Table 2 (Continued)

Mode no.	Computed val	ues	Experiment	al	Intensity		TED <sup>d</sup> (≥10%)
	Unscaled	Scaled <sup>a</sup>	FT-IR	FT-Raman	I <sub>IR</sub> <sup>b</sup>	I <sub>Raman</sub> c	
144	3203	3077			10.1	3.64	ν <sub>C27H32</sub> (28), ν <sub>C31H34</sub> (28), ν <sub>C26H30</sub> (25)
145	3209	3083			4.40	4.52	$\nu_{C15H19}$ (41), $\nu_{C18H22}$ (23), $\nu_{C20H23}$ (20)
146	3210	3084	3084m		6.31	8.84	ν <sub>C26H30</sub> (53), ν <sub>C29H33</sub> (21), ν <sub>C3H34</sub> (13)
147	3522	3384	3316s	3317w	0.16	1.76	ν <sub>N12H8</sub> (100)

 $\nu$ : stretching,  $\delta$ : bending, T: torsion, vw: very week, w: week, m: medium, s: strong, vs: very strong.

<sup>a</sup> Scaling factor: 0.9608 [28].

<sup>b</sup> Relative absorption intensities normalized with highest peak absorption equal to 100.

<sup>c</sup> Relative Raman intensities calculated by Eq. (1) and normalized to 100.

<sup>d</sup> Total energy distribution calculated B3LYP 6-31G(d,p) level, TED less than 10% are not shown.

Tal	bl	e	3
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Second order perturbation theory analysis of Fock matrix in NBO basis (PDPO).

Donor (i)	ED/e	Acceptor (j)	ED/e	$E^{(2)}$ (kJ/mol) <sup>a</sup>	E(j) - E(i) a.u. <sup>b</sup>	F(i, j) (a.u.) <sup>c</sup>
6 6	1.050	$\pi^* C_{14} - C_{16}$	0.335	19.77	0.28	0.066
$\pi c_{13} - c_{15}$	1.656	$\pi^* C_{18} - C_{20}$	0.332	20.59	0.28	0.068
6 6	1.000	$\pi^* C_{13} - C_{15}$	0.342	20.99	0.28	0.069
$\pi C_{14} - C_{16}$	1.669	$\pi^* C_{18} - C_{20}$	0.332	19.69	0.28	0.066
- 6 6	1.004	$\pi^* C_{13} - C_{15}$	0.342	19.50	0.28	0.066
$\pi c_{18} - c_{20}$	1.664	$\pi^{*}_{14}-C_{16}$	0.335	20.74	0.28	0.068
- 6 6	1.050	$\pi^* C_{26} - C_{29}$	0.327	19.32	0.28	0.066
$\pi c_{24} - c_{25}$	1.659	$\pi^* C_{27} - C_{31}$	0.330	20.60	0.28	0.068
- 6 6	1 000	$\pi^* C_{24} - C_{25}$	0.347	21.53	0.28	0.070
$\pi C_{26} - C_{29}$	1.663	$\pi^* C_{27} - C_{31}$	0.330	19.92	0.28	0.067
- 6 6	1.000	$\pi^* C_{24} - C_{25}$	0.375	19.42	0.28	0.066
$\pi C_{27} - C_{31}$	1.662	$\pi^* C_{26} - C_{29}$	0.327	20.41	0.28	0.067
		$\sigma^* C_3 - C_{24}$	0.029	0.57	1.09	0.022
$\sigma C_3 - N_{12}$	1.979	$\sigma^* C_4 - N_{12}$	0.022	0.56	1.04	0.022
		$\sigma^* C_4 - C_{13}$	0.030	2.2	1.09	0.044
		$\sigma^* C_3 - N_{12}$	0.022	0.53	1.04	0.021
$\sigma C_4 - N_{12}$	1.981	$\sigma^* C_3 - C_{24}$	0.029	2.19	1.09	0.044
		$\sigma^* C_4 - C_{13}$	0.030	0.55	1.09	0.022
		$C_2 - C_3$	0.024	1.46	0.67	0.028
		C <sub>3</sub> -H <sub>11</sub>	0.032	5.81	0.79	0.061
LPN <sub>12</sub>	1.927	C <sub>4</sub> -C <sub>5</sub>	0.033	1.49	0.68	0.029
		C <sub>4</sub> -H <sub>9</sub>	0.039	5.81	0.79	0.061
		C <sub>15</sub> -H <sub>19</sub>	0.014	0.54	0.82	0.019
		$C_1 - C_2$	0.052	0.88	1.07	0.028
LPO50(1)	1.971	C1-C5	0.063	2.56	1.07	0.047
		C <sub>36</sub> -H <sub>40</sub>	0.027	4.55	1.25	0.067
		$C_1 - C_2$	0.052	17.62	0.64	0.096
		$C_1 - C_5$	0.063	15.93	0.62	0.016
LPO(2)	1.897	$C_2 - C_3$	0.024	0.51	0.62	0.016
		$C_{36} - C_{39}$	0.032	0.55	0.68	0.018
		C <sub>36</sub> -H <sub>40</sub>	0.027	5.32	0.82	0.060

<sup>a</sup>  $E^{(2)}$  means energy of hyperconjucative interactions (stabilization energy).

 $^{\rm b}\,$  Energy difference between donor and acceptor i and j NBO orbitals.

<sup>c</sup> F(i, j) is the Fock matrix element between *i* and *j* NBO orbitals.

[27] reveals that the normal esters are characterized by the strong IR absorption due to the C=O stretching vibration in the range of  $1750-1735 \text{ cm}^{-1}$ . In this study, we have observed stretching of C=O at  $1715 \text{ cm}^{-1}$  as very strong in FT-IR and  $1714 \text{ cm}^{-1}$  as medium intense band in FT-Raman, while the computed frequency is  $1732 \text{ cm}^{-1}$  (mode no: 120) and its TED value (90%). The C-C stretching in phenyl ring and methylene chain is calculated in the range of  $1035-864 \text{ cm}^{-1}$  (mode nos: 69-64, 62, 61, 57, 55, and 52-50). These vibrations are in line with experimental values (1028, 1001, 986, 973, 889, 857: FT-IR and 1030, 1003, 988, 919 cm^{-1}: FT-Raman) and also in consistent with literature values [22,23]. These assignments are further supported by the TED values.

The identification of C–N vibration is a very difficult task, since mixing of several bands are possible in this region. However, with the help of theoretical calculation (DFT), the C–N stretching vibrations are calculated. The C–N stretching vibration coupled with scissoring of N–H, is moderately to strongly active in the region  $1275 \pm 55$  cm<sup>-1</sup> [17]. In the present investigation C–N

stretching frequencies are observed at 1046, 1056, 1068,1086 and 1110 cm<sup>-1</sup> by FT-IR and their corresponding calculated wavenumbers appeared in the range of 1049–1104 cm<sup>-1</sup> (mode nos: 70–76). These experimental values of C–N stretching mode show good agreement with theoretical values. The  $\nu$ C–N stretching vibration normally appears around 1300 cm<sup>-1</sup> [17]. In this work the  $\nu$ C–N frequencies are moderately lowered, which may be due to the mass effect around nitrogen atom.

#### 5. NBO analysis

The hyperconjugation may be given as stabilizing effect that arises from an overlap between an occupied orbital with another neighboring electron deficient orbital when these orbitals are properly orientation. This non-covalent bonding-antibonding interaction can be quantitatively described in terms of the NBO analysis, which is expressed by means of the second-order perturbation interaction energy  $(E^{(2)})$  [29–32]. This energy represents the estimation of the off-diagonal NBO Fock matrix elements. It can be deduced from the second-order perturbation approach [33]

$$E^{(2)} = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i}$$
<sup>(2)</sup>

where  $q_i$  is the donor orbital occupancy,  $\varepsilon_i$  and  $\varepsilon_i$  are diagonal elements (orbital energies) and F(i, j) is off diagonal NBO Fock matrix elements. In this present study we dealt with NBO analysis. Especially the amount of energy transfer from  $\pi$  bond orbital to anti bond  $\pi^*$  orbital, the stabilization energy  $E^{(2)}$  associated with hyperconjugative interaction, LPO(2)  $\rightarrow$  C<sub>1</sub>-C<sub>2</sub>, and C<sub>1</sub>-C<sub>5</sub> are obtained as 17.62 and 15.93 kJ/mol, respectively. The bond C<sub>13</sub>-C<sub>15</sub> with electron density 1.656e, stabilize the energy of 19.77 and 20.59 kJ/mol to its acceptor anti bonding orbitals of C<sub>14</sub>-C<sub>16</sub> and C<sub>18</sub>-C<sub>20</sub>, respectively. These interactions are observed as an increase in electron density (ED) in C-C antibonding orbital that weaken their bonds [34]. This investigation clearly demonstrates that the occupancy value of bonding orbitals make sure the hyperconjugative interaction with maximum stabilization between filled and unfilled subsystem of the molecule. The ED of  $C_{14}$ - $C_{16}$  donor bond has  ${\sim}1.669e,$  on the other hand its antibond ED ( $\pi^*$   $C_{13}{-}C_{15}$  and  $C_{18}\text{-}C_{20})$  posses  ${\sim}0.342$  and 0.332e, and their  $E^{(2)}$  energies are 20.99 and 19.69 kJ/mol respectively. From the NBO analysis, the lower the ED of donor with larger the ED of acceptor have maximum delocalization and become strong bond interaction. The higher the ED value with lower  $E^{(2)}$  energy which becomes lesser interaction and hence it shifts the vibrational frequencies from the actual frequencies. It is evident that the  $C_3-N_{12}$  (1.979e) and  $C_4-N_{12}$  (1.981e) bond stretching vibration (in the range from 1049 to 1123; mode nos. 70-76) lowers from the normal C-N bond stretching (1300 cm<sup>-1</sup>) [17]. This may be due to the lesser hyperconjugative interaction between C-N donor bonds to C-C acceptor bands. The  $E^{(2)}$  values and types of the transition are shown in Table 3.

# 6. HOMO-LUMO

The frontier molecular orbitals play an important role in the electric and optical properties, as well as in UV-vis spectra and chemical reactions [35]. The analysis of the wave function indicates that the electron absorption corresponds to the transition from the ground to the first excited state and is mainly described by one electron-excitation from the highest occupied molecular orbital (HOMO) to the lowest unoccupied orbital (LUMO) [36]. The energy gap for PDPO was calculated using B3LYP/6-31G(d,p) level. The bioactivity and chemical activity of the molecule depends on the eigen value of HOMO, LUMO and energy gap. LUMO as an electron acceptor represents the ability to obtain an electron; donor represents the ability to donate an electron. The frontier molecular orbitals are shown in Fig. 5. From the molecular orbital analysis the highest occupied level is 87 this locates over the C-N-C group. And the 88 is the excited frontier orbital (LUMO- $\pi^*$ ), this orbital located over the C<sub>1</sub>-O<sub>50</sub> and carbon atoms in phenyl ring. The energy difference between the HOMO and LUMO is about 5.288 eV. The frontier molecular orbital of PDPO (HOMO-LUMO) is shown in Fig. 5.

HOMO energy = -6.169 eV

LUMO energy = -0.881 eV

Energy gap = 5.288 eV

The smaller band gap energy increases the stability of the molecule. The charge distribution of the molecule has calculated



LUMO (-0.881 eV)

Fig. 5. The frontier molecular orbital of PDPO (HOMO-LUMO).

**Table 4**Atomic charge of PDPO.

Atoms	Charges (a.u.)	Atoms	Charges (a.u.)
C <sub>1</sub>	0.402	C <sub>24</sub>	0.099
C <sub>2</sub>	-0.226	C <sub>25</sub>	-0.118
C <sub>3</sub>	-0.011	C <sub>26</sub>	-0.092
C <sub>4</sub>	0.022	C <sub>27</sub>	-0.088
C <sub>5</sub>	-0.119	C <sub>29</sub>	-0.099
N <sub>12</sub>	-0.515	C <sub>31</sub>	-0.079
C <sub>13</sub>	0.060	C <sub>35</sub>	-0.178
C <sub>14</sub>	-0.113	C <sub>36</sub>	-0.198
C <sub>15</sub>	-0.107	C <sub>39</sub>	-0.173
C <sub>16</sub>	-0.092	C <sub>42</sub>	-0.180
C <sub>18</sub>	-0.090	C <sub>47</sub>	-0.318
C <sub>20</sub>	-0.082	O <sub>50</sub>	-0.465

using B3LYP/6-31G(d,p) level. This calculation depicts the charges of the every atom in molecule. Distribution of positive and negative charges is the cause, to increase or decrease of bond length. The atomic charges of carbon, nitrogen and oxygen are listed in Table 4, in which nitrogen atom has maximum negative charge of -0.515 and -0.465 a.u., for oxygen atom. The HOMO part is located over the N<sub>12</sub>-C<sub>3</sub>, N<sub>12</sub>-C<sub>4</sub> orbital, is mainly due to the lone pair of electron. Some of the carbon atoms have only positive charge about C<sub>1</sub> (0.402), C<sub>4</sub> (0.022), C<sub>13</sub> (0.060) and C<sub>24</sub> (0.099 a.u.). This clearly explains that the LUMO exist in those areas. The Mulliken charge plot is shown in Fig. 6.



Fig. 6. Mulliken charge plot of C, N, O in PDPO.

# 7. Conclusion

All possible conformers are calculated by changing the torsion angle rotation with respect to bond. The calculated bond parameters are compared with reported X-ray diffraction data. All the vibrational bands which are observed in the FT-IR and FT-Raman spectra of the title compound are completely assigned for the first time with the help of TED. The donor–acceptor interaction, as obtained from NBO analysis could fairly explains the decrease of occupancies of  $\sigma$  bonding orbital and the increase of occupancy of  $\pi^*$  antibonding orbitals. The bioactivity of the molecule is proposed by means of band gap (–5.288 eV) energy derived from HOMO and LUMO calculation. The atomic charges of the present molecule has been calculated and also plotted.

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