

Raman and IR spectra of graphdiyne nanoribbons

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Abstract

γ -graphdiyne is a 2D carbon structure beyond graphene: it is formed by sp and sp^2 carbon atoms organized as hexagonal rings connected by linear links, and it is predicted to be a semiconductor. The lateral confinement of γ -graphdiyne nanoribbons significantly affects the electronic and vibrational properties. By means of periodic Density Functional Theory (DFT) calculations we here investigate the electronic band structure, the Raman and IR spectra of γ -graphdiyne 2D crystal and related nanoribbons. We discuss the effect of the functional and basis set on the evaluation of the band gap, highlighting the reliability of hybrid functionals. By joining DFT calculations with a symmetry analysis, we assign in detail the IR and Raman spectra of γ -graphdiyne. On this basis we show the modulation of the gap in nanoribbons of increasing width and different edges (armchair, zigzag). We assess how confinement affects the Raman and IR spectra by comparing vibrational modes with phonons of the parent 2D crystal. Our symmetry-based classification allows identifying the marker bands sensitive to the edge structure and lateral confinement of nanoribbons of increasing width. These results show the effectiveness of vibrational spectroscopy for the characterization of such nanostructures.

1. Introduction

Carbon materials and their nanostructures played a relevant role in the science and technology of the last two decades: from fullerenes to carbon nanotubes, from polyconjugated polymers to graphene, the so-called “era of carbon allotropes” has been enlightened by groundbreaking results, paving the way to many interesting research topics [1]. In the last years, the interest of many scientists has been directed towards exotic forms of carbon, including systems based on sp-hybridized carbon (variously referred to as carbyne, carbon-atom wires, polyynes, cumulenes, ...) or hybrid sp-sp² or sp-sp³ nanostructures [2-6], focusing both on their fundamental properties and on their potential interest for applications.

Research on sp-carbon systems dates back to the end of XIX century and the first theoretical investigation of sp-sp² carbon systems (*e.g.*, graphyne GY and graphdiyne GDY) has been published in 1987 [7]. The advent of graphene and related materials strongly renewed the interest in these peculiar systems, also from the experimental point of view [8-10]. In fact, GY and GDY can be considered as possible modification of graphene, where novel 2D crystals are formed by interconnecting sp²-carbon hexagons with sp-carbon chains of different lengths, and show the occurrence of Dirac cones in their electronic structure [11, 12].

Bottom-up approaches have been successfully employed to produce sub-fragments of GDY of different topology and dimension. In particular, Haley's group has been very active in synthesizing a variety of molecules mimicking GDY [13-17]. More recently, different papers reported the preparation and characterization of extended 2D GDY sheets by means of organometallic synthesis techniques, showing promising routes to the production of these systems, even though significant efforts should still be put to further investigate and understand their properties [18-20]. Among these hybrid sp-sp² carbon nanostructures, the γ polymorph of GY and GDY is the system that attracted the widest attention both from the experimental and theoretical points of view.

In addition to the limited experimental work, a much larger amount of papers focused on the prediction of the properties of GDY (and related systems such as GDY nanoribbons, hereafter referred to as GDYNRs) mainly through Density Functional Theory (DFT) calculations [5,6,21-24].

Among the most important features of GDY, the electronic band structure and band gap have been investigated in detail, including also the study of confinement effects in GDYNRs or defected systems. Due to the relevance of this family of hybrid sp-sp² carbon materials in current nanoscience and nanotechnology, effective characterization tools with a combined experimental/computational approach are mandatory for a detailed investigation of these systems.

Vibrational spectroscopy is extremely useful to characterize carbon-based materials and Raman in particular has been employed in the first experimental works reporting the preparation of GDY-based materials [25-29].

Despite the effectiveness of these spectroscopic techniques up to now and to our knowledge, only few investigations focused on the prediction of the vibrational properties of GDY [27-29], . Popov *et al.* computed the Raman spectrum of different polymorphs of GY [26], Zhang *et al.* gave an assignment of the Raman spectrum of GY and GDY and studied the effects of strain by Raman [27]. Wang *et al.* discussed the Raman spectra of different finite-size models of different sp-sp² carbon nanostructures [29] while IR active C \equiv C stretching band has been discussed in Ref. [28].

However, a basic description of the vibrational dynamics of GDY is lacking. Similarly, the effects of delocalization vs. confinement on the spectra of GDYNRs call for an investigation of the spectroscopic markers useful for the characterization of nanoribbons with different width and edge topology. Even if the experimental spectra of these material are not available so far, we believe that the theoretical study of their vibrational states can highlight several aspects related to the peculiar electronic and

molecular structure of GDY and GDYNRs, and to the effectiveness of vibrational spectroscopy techniques for molecular recognition and characterization.

Here, we have computed the electronic structure of 2D-GDY by periodic DFT simulations (CRYSTAL code) adopting different functionals and basis sets. Thereafter, we have focused on the prediction and assignment of IR and Raman spectra. We have analyzed GDYNRs as a function of the nanoribbon width and edge-type (armchair or zigzag), disclosing the modulation of the band gap, and peculiar markers in IR and Raman that are sensitive to the lateral confinement and to the molecular structure of the edges.

2. Computational Details

Geometry optimization, band gap evaluation and prediction of IR and Raman spectra have been carried out for the two-dimensional (2D) crystal γ -GDY (also called (6,6,6)-graphdiyne and hereafter referred as 2D-GDY) and for GDYNRs, treated as one-dimensional (1D) crystals, by employing DFT simulations and applying Periodic Boundary Conditions in two and one dimensions respectively. The CRYSTAL17 code [30, 31] has been adopted to this aim, exploiting the possibility to employ hybrid exchange-correlation functionals together with Gaussian basis sets.

In the case of 2D-GDY, for which reference theoretical data are already available in the literature both considering band gaps [5, 6] and Raman spectra [27], LDA (VWN), GGA (PBE and BLYP) and hybrid functionals (PBE0, HSE06, B3LYP) have been considered with 6-31G(d,p) basis sets. For PBE0 and HSE06 only, also the more extended Ahlrichs VTZ + Polarization basis set [32] has been used. This allowed analyzing the reliability of different functionals, including hybrid ones, and the influence of basis set in the prediction of the band gap.

PBE0/6-31G(d,p) and HSE06/6-31G(d,p) levels of theory have been then chosen to predict the gap of the different GDYNRs of different width, while, among these, Raman spectra could be computed only at PBE0/6-31G(d,p) level in CRYSTAL17 since HSE06 is not yet implemented for Raman response. Our previous experience in the prediction of the Raman response of several sp-carbon based molecular systems shows that this functional provides a good agreement vs. experimental data [33-35]. According to the discussion reported in Ref. [36], the exponent of the diffuse sp orbitals in 6-31G(d) basis set of carbon atoms have been increased from 0.1687144 Bohr⁻² to 0.187 Bohr⁻² to avoid convergence problems in the SCF cycles, due to basis sets linear dependencies. For the same reason, when using the VTZ basis set, the exponent 0.12873135 Bohr⁻² of one the s function and the exponent 0.10084754 Bohr⁻² of one the p functions have been changed to 0.153 and 0.12 Bohr⁻² respectively.

Considering other parameters of the CRYSTAL simulations, the tolerance on integral screening (TOLINTEG parameters) have been fixed to 9,9,9,9,80, while the shrink parameters defining Monkhorst-Pack sampling points have been fixed to 100 for the calculation of the band structures and gaps and 50 for the vibrational analysis. In both case, full convergence on the total energy had been obtained.

Since, in absence of experimental data, the comparative analysis here presented concerns calculated spectra, it does not require the usually adopted scaling of the transition frequencies. The paper reports unscaled wavenumber values both in the discussion and in the Figures: a suitable scaling factor could be defined [37] whenever comparing these theoretical spectra with experimental ones.

3. Results and Discussion

To present the results coming from DFT calculations of 2D-GDY and of three series of nanoribbons, we refer to the nomenclature introduced in previous papers [5, 6, 21-23]. Armchair and zigzag are indicated by A(*n*)-GDYNR and Z(*n*)-GDYNR, respectively, where the index *n* refers to the width of

GDYNR, which is an integer value for A(n)-GDYNR ($n = 1, 2, \dots 5$) and integer or half integer value in the case of Z(n)-GDYNR ($n = 1, 3/2, \dots 5$), as depicted in Figure 1. Such GDYNRs models can be classified according to the proper line-symmetry groups, isomorphs to D_{2h} group in the case of A(n)-GDYNRs and Z(n)-GDYNRs with half integer n . Z(n)-GDYNRs with integer n , belong to the C_{2v} group.

For all GDYNRs, hydrogen atoms have been added at the edges as end-groups, in agreement with most of the previous computational works [5, 6, 21-23]. This choice is reasonable also from the experimental point of view, based on the finite GDY fragments that have been synthesized in the past [17]. To assess the influence of the edge type on both electronic and vibrational properties, we have considered also the A(1) and Z(1) systems, which correspond to co-polymers formed by alternated diacetylenic and phenyl-rings units connected respectively in para- and meta- positions [38]. These two limiting cases represent a reference system formed by just the edge of A(n)- and Z(n)-GDYNRs.

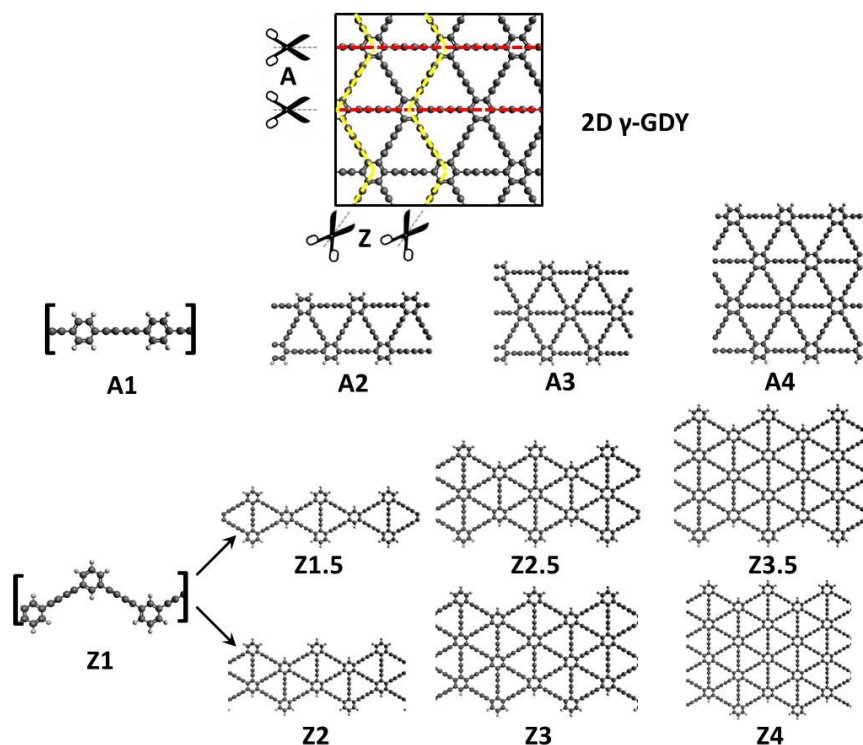


Figure1: Sketches of the armchair (A_n) and zigzag (Z_n)-GDYNRs investigated in this work. n is the index representing the nanoribbon width.

The lattice parameters and fractional coordinates of the optimized structure of all the systems here investigated are reported in the Supplementary Material [50], including the computed wavenumbers, IR intensities, Raman activities, and graphical representations of the normal modes of 2D-GDY and of the main GDYNR markers discussed in the text.

3.1 Electronic properties of 2D γ -graphdiyne and its nanoribbons

As in the case of other carbon-based polyconjugated materials, the correct prediction of the gap suffers from the limitations of current DFT pure functionals in describing accurately π -electron delocalization, with a tendency to overestimate its effect, thus causing unrealistically low predictions of the band gap. For instance, the gap of 2D γ -GDY reported in the literature changes from about 0.4 eV (LDA), 0.5 eV (GGA) to 0.9 - 1.1 eV when employing hybrid functionals or the GW method. The

latter values are considered more reliable [5, 6, 12, 24]. In fact, it is well-known that hybrid functionals significantly improve the accuracy in the description of π -electron delocalization, but their use is not convenient when employing plane waves and pseudopotential methods to carry out DFT calculations in periodic systems. A useful alternative is provided by Gaussian basis sets, which allow to use hybrid functionals at an acceptable computational cost: this approach is implemented in the CRYSTAL code [30-31] which offers the valuable opportunity to extend to infinite systems the same computational approach typical of finite molecular systems.

As illustrated in previous papers [5, 6], the gap in the band structure of γ -GDY is found at the Γ point (Figure 2).

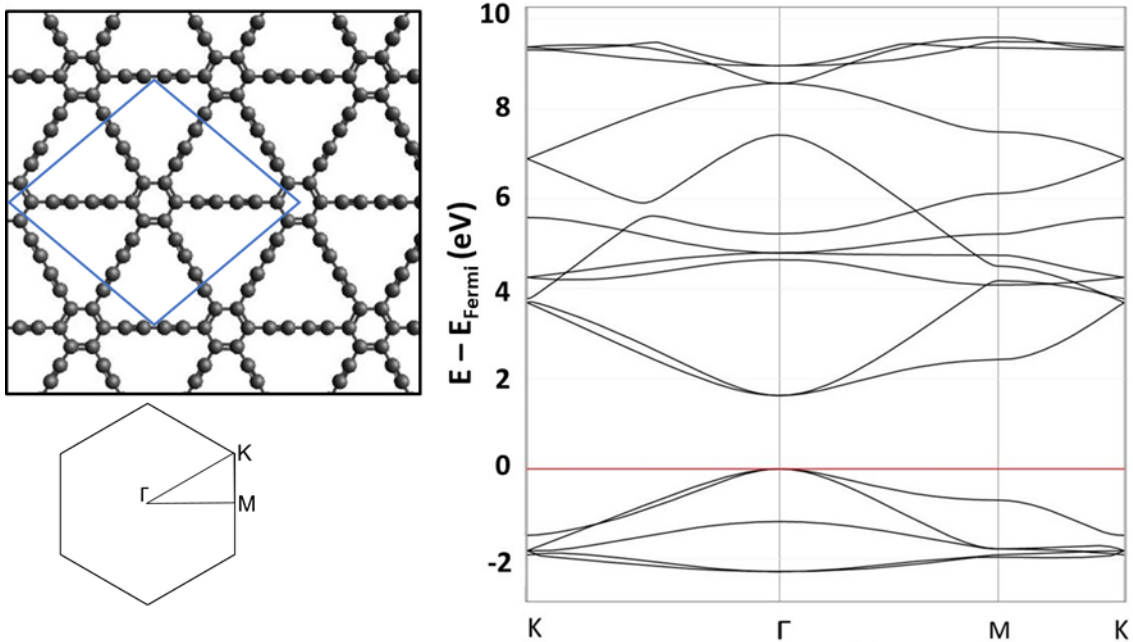


Figure 2: Electronic band structure of 2D-GDY (PBE0/6-31G(d) DFT calculation).

We report in Table 1 the band gap computed by employing different LDA, GGA and hybrid functionals. For PBE0 and HSE06 we also provide the comparison of the results produced by a double- ζ basis set (6-31G(d)) vs. a triple- ζ basis set (VTZ). We note that the effect of the basis set is less important than the choice of the functional: indeed, both for PBE0 and HSE06, adopting the more accurate VTZ basis set gives in both cases a gap which is just about 0.05 eV larger than the values obtained with 6-31G(d) basis set. Therefore, we can suppose that the latter basis set is sufficiently accurate to model the properties of this system.

Table 1: Band gaps of 2D-GDY computed by employing different exchange-correlation functionals and gaussian basis sets (see text for details).

XC functional	Basis set	Band Gap (eV)
PBE0	6-31G(d)	1.63
	VTZ	1.67

HSE06	6-31G(d) VTZ	1.11 1.16
B3LYP	6-31G(d)	1.40
BLYP	6-31G(d)	0.48
PBE	6-31G(d)	0.45
LDA (VWN)	6-31G(d)	0.40

Considering LDA and GGA functionals (PBE, BLYP), we obtain band gaps of 0.4 (LDA), 0.45 (PBE) and 0.48 eV (BLYP), in full agreement with previous calculations. As expected, hybrid functionals provide higher values of the band gap: 1.6 eV (PBE0), 1.4 eV (B3LYP) and 1.1 eV (HSE06). The latter value agrees with the result of GW calculations, usually taken as an accurate reference value. This also agrees with the fact that HSE06 has been found to give a more accurate prediction of band gaps with respect to the parent PBE0 functional [39].

Considering zigzag and armchair GDYNR, in Figure 3 we plot the band gap of A(n)-GDYNRs and Z(n)-GDYNRs as a function of the n index ($n \leq 5$) and compared with the values found for 2D-GDY (*i.e.*, $n \rightarrow \infty$).

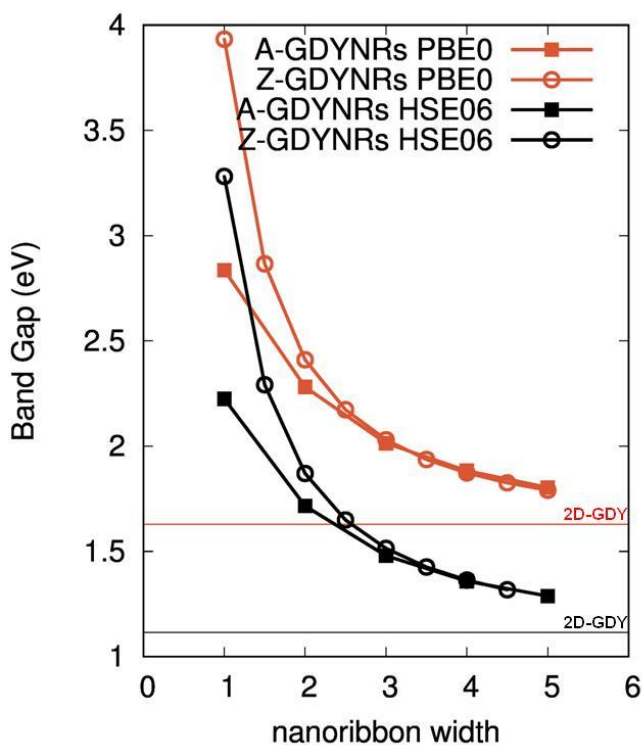


Figure 3: Band gap (eV) of armchair and zigzag GDYNR as a function of width index (n) as obtained by PBE0/6-31G(d) (in red) and HSE06/6-31G(d) (in black) calculations. Numerical values of these band gaps are reported in Table S2 of the Supplementary Material [50]. The value band gap of 2D-GDY is also indicated as a comparison by the horizontal lines.

Several works report that the gap of confined GDY is larger than the gap of the infinitely extended 2D GDY and decreases for increasing size, towards the limit of 2D-GDY [5, 6, 21-23]. Confinement effects

caused by the finite width of GDYNRs (n) modulate the gap, similar to the behavior of graphene nanoribbons with respect to the graphene crystal. As show in Figure 3 this modulation of the gap spans a range of about 1 eV (for $n \geq 2$). As expected, the values obtained with the HSE06 functional are systematically lower than those obtained with PBE0. However, both functionals essentially describe the same behavior.

Interestingly, while for $n > 3$ the trends are the same for both edges, for small widths ($n < 3$), Z(n)-GDYNRs have a larger gap with respect to A(n)-GDYNRs. The reason for this is evident if we consider the gap values obtained for the limiting case ($n = 1$) of the 1D polymers A(1) and Z(1) (Figure 1). Both polymers can be described as sp-carbon segments of four carbon atoms (*i.e.*, diacetylenic units) interconnected by phenyl rings. The connection on these rings can be done along three different conjugation paths, corresponding to para-, meta- and ortho- connections. As highlighted by Tahara et al. investigating the case of graphyne fragments [38], A(1) corresponds to a para-conjugated system where the delocalization of π -electrons along the system occurs more efficiently, thus promoting the lowest gap. Conversely, the meta-conjugation characteristic of Z(1) reduces π -electron delocalization, which justifies the higher band gap. As expected, the influence of the edge type is effective for small widths, but rapidly decreases for increasing width. For $n > 3$ the edge type (A- or Z-) has a very limited influence on the gap, even if the gap remains still quite far from the $n \rightarrow \infty$ limit of the 2D-GDY crystal.

3.2 Vibrational spectra and optically active phonons of 2D γ -GDY

The phonons of 2D-GDY at the Γ point can be classified according to the D_{6h} point group, which is isomorphic to the P6/mmm layer group of the crystal. The structure of the representation of the D_{6h} point group in the vibrational space is:

$$\Gamma^{\text{vib}} = 3A_{1g} + 2A_{2g} + 3B_{2g} + 3E_{1g} + 6E_{2g} + 2A_{2u} + 5E_{1u} + 3B_{1u} + 3B_{2u} + 3E_{2u}.$$

A_{1g} , E_{1g} and E_{2g} phonons are Raman active, whereas A_{2u} and E_{1u} are IR active; the rest of the irreducible representations (A_{2g} , B_{2g} , B_{1u} , B_{2u} , E_{2u}) are inactive. Therefore, 12 peaks (9 of which are double-degenerate), are expected in the first-order Raman spectrum, and 7 absorption bands (5 double-degenerate) in the IR spectrum. Furthermore, since the D_{6h} point group possesses inversion symmetry, there is mutual exclusion between IR and Raman transitions. the Raman and IR spectra of 2D-GDY computed by DFT are reported in Figure 4.

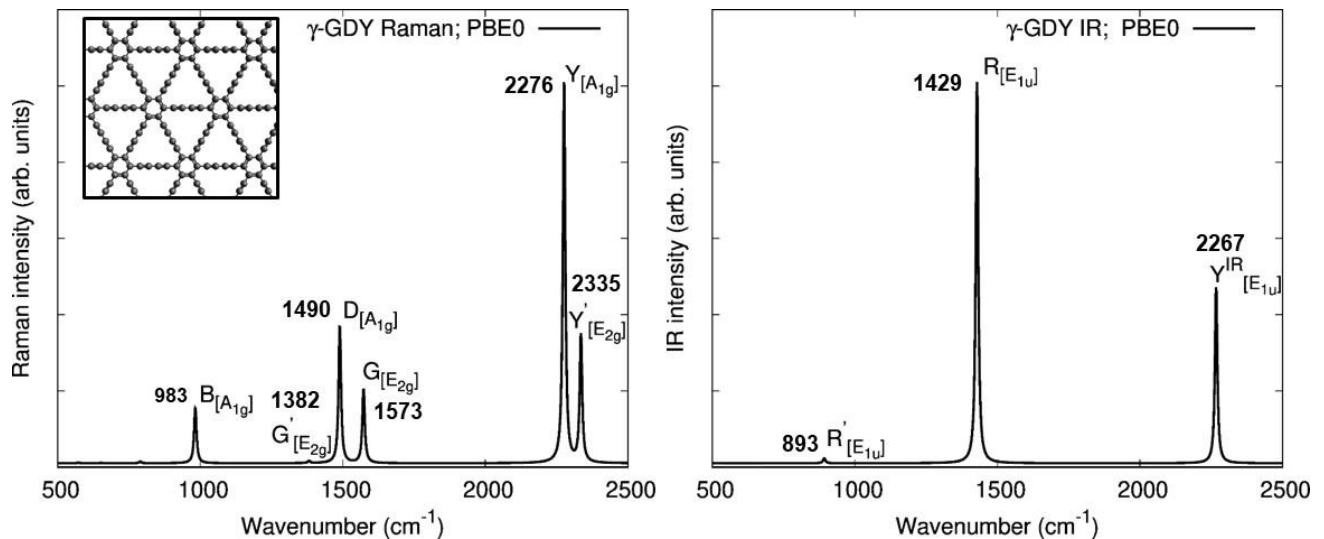


Figure 4: DFT computed (PBE0/6-31G(d)) Raman and IR spectra of 2D-GDY. The wavenumber values are not scaled.

Our calculations provide a pattern of the Raman spectrum which is similar to the one determined by Zhang *et al.* adopting LDA and plane wave pseudopotential method [27]. The labels used in Figure 4 to identify the different Raman lines have been chosen analyzing the related vibrational eigenvectors, to suggest possible correlations with the vibrational transitions of related materials (e.g., G and D Raman lines of graphene).

Table A of the Appendix (reported in the Supplementary Materials [50]) shows the basis set of the stretching coordinates and the symmetry-adapted vibrational coordinates defined accordingly. The high symmetry of 2D-GDY allows to draw several conclusions on the vibrational displacements of individual phonons at Γ , and to obtain information about allowed and forbidden dynamical couplings among vibrational coordinates. The behavior based on the analysis of symmetry coordinates is general, and independent from the level of theory adopted for spectra simulations.

The analysis presented here is limited to CC stretching internal coordinates: indeed, in 2D-GDY, CC stretching modes dominate the vibrational spectra above 1000 cm^{-1} , giving rise to the strongest Raman and IR transitions. Crystal redundancies and several local redundancies (*i.e.*, ring redundancies) [40, 41] involve both bending and stretching coordinates, thus intrinsically determining a coupling among bending and stretching displacements. However, we can obtain a sound description of the most relevant normal modes, limiting the analysis to their stretching component.

3.2.1 CC stretching symmetry coordinates.

The following internal coordinates belonging to the reference unit cell (Table A) allow describing the CC stretching subspace:

- 1) six equivalent CC stretching of the aromatic ring, $\{R_i; i = 1 \dots 6\}$
- 2) CC stretching of the bonds of the six polyyne arms. Each arm contributes to the reference cell with one half of its bonds, whose stretching coordinates are described by three sets, namely: $\{r_i; i = 1 \dots 6\}$, $\{T_i; i = 1 \dots 6\}$, and $\{P_i; i = 1 \dots 3\}$. r_i refers to “single” bonds linked to the aromatic unit, T_i are “triple” bonds stretching, and P_i are the stretching coordinates of the central CC bonds, which carry inversion centers. Each P_i is shared with an adjacent crystal cell, so that only three P_i coordinates are associated to the reference cell.

To highlight correlations with the normal modes of a simple diphenyl-polyyne molecule it is very useful to adopt a description of the phonons using the displacement patterns involving the six polyyne arms (actually diynes, each consisting of 5 CC bonds). This description is obtained by introducing the group symmetry coordinates of the individual polyyne chains (Table A.2). Accordingly, we obtain the following sets of equivalent coordinates; every set contains the six group coordinates associated to each polyyne arm:

$$\{r_i^+\}, \{r_i^-\}, \{T_i^+\}, \{T_i^-\}, \{P_i\}$$

Thanks to translational symmetry, it is immediate to verify that the sets $\{r_i^+\}$, $\{T_i^+\}$, and $\{P_i\}$ are involved in phonons of “gerade” symmetry (Raman active). IR active “ungerade” phonons do involve $\{r_i^-\}$ and $\{T_i^-\}$. According to D_{6h} symmetry, each set gives symmetry coordinates belonging to A_{1g} , E_{2g} , B_{2u} and E_{1u} species, as described below.

(a) the A_{1g} subspace is spanned by 4 A_g symmetry coordinates. These correspond to the in-phase combinations of the internal (or group) coordinates belonging to the different sets, which originate

the symmetry coordinates $A_{1g}^R, A_{1g}^{r+}, A_{1g}^{T+}, A_{1g}^P$ defined in Table A.3. It is important to note that the 3 A_{1g} Raman active phonons are linear combinations of these four A_{1g} symmetry coordinates and the four dimensional A_{1g} subspace contains a crystal redundancy (*i.e.*, the in-phase combination of the four A_{1g} stretching coordinates, which describes a simultaneous stretching of all CC bonds belonging to each cell, and which would imply a change of the crystal volume).

(b) 4 phonons belonging to the E_{2g} subspace can be described as linear combinations of the 4 E_{2g} symmetry coordinates ($E_{2g}^R, E_{2g}^{r+}, E_{2g}^{T+}, E_{2g}^P$). The remaining 2 E_{2g} phonons predicted for 2D-GDY can be accounted for by introducing bending coordinates.

(c) 3 phonons of the E_{1u} subspace are linear combinations of the 3 symmetry coordinates $E_{1u}^R, E_{1u}^{r-}, E_{1u}^{T-}$ (P_i coordinates cannot appear in *ungerade* species because each P_i bond carries an inversion center). The remaining 2 E_{1u} phonons are expected to involve mainly bending displacements.

(d) B_{2u} is the last symmetry species involving stretching coordinates, and it is associated to phonons inactive in the vibrational spectra. It contains 3 phonons which are linear combinations the B_{2u} symmetry coordinates $B_{2u}^R, B_{2u}^{r-}, B_{2u}^{T-}$. Based on the structure of the representation, we expect one further B_{2u} phonon associated to bending displacements.

A_{2u} IR-active phonons and E_{1u} Raman-active phonons cannot be described by the chosen basis set made of just stretching coordinates: according to the character table, A_{2u} and E_{1u} phonons must involve out-of-plane displacements, such as those associated to out-of-plane bending and torsions. For this reason, such phonons are expected to lie in the low-wavenumber region of the IR spectrum (indeed, the A_{2u} transitions are computed by CRYSTAL at 183 and 485 cm^{-1} and the E_{1g} transitions are computed at 137 and 474 cm^{-1} , showing in both cases a negligible intensity in the IR or Raman spectrum, see Supplementary Material [50])

DFT calculations supply the nuclear displacements of the phonons, which are used to draw the graphical representation of the vibrational patterns associated to the most relevant Raman and IR bands (see Supplementary Material [50]). The inspection of these graphics provides a description of such phonons as linear combinations of the symmetry coordinates introduced above.

3.2.2 Raman and IR assignment

It is well-known that the marker bands of sp-hybridized CC bonds are found in the 2000-2500 cm^{-1} range [2, 25]. Indeed, the Y and Y' phonons are respectively A_{1g} and E_{2g} collective CC stretching vibrations localized on the sp-carbon domains of GDY. The combination of the r_i^+, T_i^+, P_i coordinates of each i -th polyyne arm follows the characteristic pattern shown by the Effective Conjugation Coordinate (ECC) mode of polyynes, described as a collective simultaneous $\text{C}\equiv\text{C}$ stretching/C-C shrinking of the bonds forming the chain (r_i^+ and P_i oscillate in phase, while T_i^+ vibrate out-of-phase). The properties of this mode have been widely discussed in the past [2, 25], extending the treatment of vibrational dynamics developed for polyconjugated polymers a few decades ago [42-44]. In the A_{1g} Y mode (2276 cm^{-1}), all sp-carbon chains oscillate in-phase, according to the ECC coordinate. In the E_{2g} Y' mode (2335 cm^{-1}) the ECC vibrational pattern is repeated on the 6 polyyne segments with different relative phases, according to E_{2g} symmetry. The sizeable difference in wavenumber of these two phonons (59 cm^{-1}) indicates a non-negligible coupling among adjacent

polyyne chains, caused by the interaction among the π electrons of the phenyl unit and of the attached sp-chains. This is supported by the calculation of the vibrational structure of a di-phenyl polyyne consisting of a linear chain having 4 sp-hybridized carbon atoms capped with two phenyl groups (*i.e.*, the smallest structural unit defining GDY). The ECC mode of such model molecule is computed at 2368 cm^{-1} , much higher than the Y and Y' bands of GDY. This proves the occurrence in GDY of significant π electron delocalization across phenyl groups (see Supplementary Material [50]).

The region below 1600 cm^{-1} is commonly assigned to stretching vibrations of the aromatic rings. However, phonons involving R_i coordinates, always show a remarkable coupling with “single” bonds stretchings of the polyyne arms (r_i and P_i).

The phonons of A_{1g} symmetry are associated to the following Raman bands:

- the D line (1490 cm^{-1}) is assigned to a phonon described as the A_{1g}^R ring breathing coupled to A_{1g}^{r+} coordinates, namely to the stretchings of the CC bonds linked to the aromatic moiety. The A_{1g}^R and A_{1g}^{r+} coordinates vibrate out of phase, with a pattern very similar to that of the phonon associated to the D line of graphite/graphene. The A_{1g}^P coordinate is also involved, to a lesser extent.
- the B line (983 cm^{-1}), associated to the breathing mode of the phenyl units, out-of-phase coupled with the A_{1g}^P coordinate. The A_{1g}^{r+} coordinate is also involved, with a minor contribution.

Symmetry selection rules for A_{1g} phonons tell us that only the three diagonal elements of the Raman polar tensor, namely ($\alpha_{xx} = \alpha_{yy}, \alpha_{zz}$) are non-vanishing. According to the calculations (see SI), all relevant Raman transitions listed above show a negligible out-of-plane α_{zz} component. So, the intensity of these Raman lines are determined by the value $|\alpha_{xx}|^2 = |\alpha_{yy}|^2$. This implies that for 2D-GDY sheets deposited on a substrate (x, y plane), Raman experiment in backscattering geometry at normal incidence (z direction) will provide the same intensity pattern, independently on the polarization of the incident and scattered light, because the symmetry of the Raman tensors does not allow assessing the orientation of the sheet in the x, y plane. A proof of the orientation of the sheet with respect to the substrate should be obtained with normal incidence and collection of the scattered photons at 90° (e.g. x direction). In this case A_{1g} bands should vanish for z-polarization of the scattered photons.

The E_{2g} Raman transitions are the following:

- the G mode (1573 cm^{-1}): it involves E_{2g}^R coordinate of the phenyl units with in phase contribution by E_{2g}^{r+} coordinate. The displacements pattern recalls that associated to the G line of graphene.
- the weak G' mode (1382 cm^{-1}); it also involves the E_{2g}^R coordinate of the phenyl unit, as the G mode; the contribution from the polyyne chain involves E_{2g}^P coordinate and, to a lesser extent, E_{2g}^{r+} .
- A very weak E_{2g} bands at 790 cm^{-1} , corresponding to another different linear combination of E_{2g}^R, E_{2g}^{r+} and E_{2g}^P coordinates, with non-negligible bending contributions.
- two very weak bending phonons ($573\text{ cm}^{-1}, 394\text{ cm}^{-1}$).

Considering a degenerate pairs for each E_{2g} phonons, the nonvanishing elements of the Raman tensor are $\alpha_{xx} = -\alpha_{yy}$ and α_{xy} respectively, with $|\alpha_{xx}|^2 = |\alpha_{xy}|^2$.

Accordingly, the polarization properties of the E_{2g} bands of 2D-GDY sheets deposited on a substrate result to be the same as for A_{1g} transitions: for backscattering geometry, one expects independence of the Raman intensity vs. the polarization direction within the xy plane.

In the IR spectrum, since the 2 A_{2u} modes practically show almost zero intensity (see Table S5 in the

Supplementary Material [50]) we essentially observe E_{1u} phonons, namely:

- the Y^{IR} band (2267 cm^{-1}) assigned to the out-of-phase combination of E_{1u}^{r-} and E_{1u}^{t-} coordinates; focusing on individual polyyne arms, it can be described as the ECC mode with a node, located on the central CC bond;
- the R band (1429 cm^{-1}), which is mainly due to CC stretching of the bonds in the phenyl units (E_{1u}^R) with out-of phase contribution of the E_{1u}^{r-} coordinate;
- the very weak R' transition (893 cm^{-1}); it mainly involves the E_{1u}^R coordinate (as the R band), coupled in-phase with the E_{1u}^{r-} coordinate; a careful inspection of the vibrational patterns shows that a non-negligible contribution by bending displacements affects the R' phonon;
- two very weak bending phonons are computed at 419 cm^{-1} and 171 cm^{-1} .

Considering a degenerate pair for each E_{1u} phonon, the non-vanishing elements of the associated dipole derivatives are μ_x and μ_y respectively, with $|\mu_x|^2 = |\mu_y|^2$. The above relationship tells us that IR experiment with polarized light at normal incidence on the GDY plane cannot discriminate between oriented and un-oriented sheets in the plane.

The assignments here reported are the starting point for the discussion of the spectra of GDYNRs, and allow to discriminate among phonons characteristic of the bulk and phonons localized on the edges, which can be taken as markers of the spatial confinement.

3.3 Raman and IR spectra of GDYNRs: markers of confinement

The detailed analysis of Raman and IR spectra of A- and Z- nanoribbons presented here aims at discussing the existence of marker bands that could be taken as signature of spatial confinement and/or edge type (A- or Z-).

3.3.1 Raman spectra

Figure 5 compares Raman spectra of A(n)- and Z(n)-GDYNR for increasing widths with the spectrum of 2D-GDY, discussed in the previous section. Starting from $n = 2$, both A(n)- and Z(n)-GDYNRs show strong bands which can be put in correspondence with the Raman bands of 2D-GDY. We discuss bands in the region of sp-carbon diacetylenic segments ($2000\text{-}2300\text{ cm}^{-1}$ range) and in the region of sp² carbon of the phenyls ($1400\text{-}1600\text{ cm}^{-1}$ range).

2000-2500 cm^{-1} region. A strong doublet ($\approx 2300\text{ cm}^{-1}$) correlates with the Y and Y' lines of 2D-GDY. The strongest A_{1g} band starts from 2307 cm^{-1} (2305 cm^{-1}) in A(2)-GDYNR (Z(2)-GDYNR), and in larger ribbons converges to a unique wavenumber (2285 cm^{-1} , about 10 cm^{-1} higher than Y line of 2D-GDY, and independent on edge topology – see Figure 5). The remarkable frequency dispersion ($\approx 30\text{ cm}^{-1}$) from $n = 2$ to $n = \infty$ (2D-GDY) suggests that this band is highly sensitive to π electron delocalization, thus indicating that there is a strong interplay between the π electrons of the polyyne arms and those of the aromatic rings. The effect of edge topology on the Y line can be appreciated only considering very thin ribbons ($n = 1, 1.5$).

The higher wavenumber component of such doublet correlates with the Y' E_{2g} line of 2D-GDY, and shows a less pronounced dispersion (10 cm^{-1} for A(n)-GDYNRs and 20 cm^{-1} for Z(n)-GDYNRs) while it is more sensitive to the edge type.

In the case $n = 1$, the Y-Y' doublet merges in a single band predicted at 2344 cm^{-1} and 2371 cm^{-1} for A and Z species, respectively. This band corresponds to the ECC mode of the single unit of polyyne (one-

unit cell) in the sp-carbon segment. Remarkably, the wavenumber of this mode in A(1)-GDYNR is significantly lower than the corresponding mode of the di-phenyl-polyyne model molecule (2368 cm^{-1}), while it almost coincides for Z(1)-GDYNR. This complies with the effect of conjugation between π electrons of the polyyne chain and π electrons of the aromatic ring being more effective in the case of the para-substitution (see the discussion above on the band gaps). A thorough discussion on the physical effects ruling this behavior can be found in Ref. [35].

The lowering of symmetry in GDYNRs with respect 2D-GDY concurs to the activation of different modes, close in frequency and mainly contributing to the two main Y and Y' bands. Sometimes, weak additional bands can be identified (*e.g.*, A(4), A(5), Z(2), Z(4)).

The Y-Y' doublet cannot be taken as characteristic marker of a ribbon, because of its clear relationship with the corresponding doublet of the 2D crystal. However, the remarkable redshift observed with increasing width for both families of GDYNRs (Figure 5) suggests that the position of Y and Y' could be a diagnostic tool regarding the width of GDYNRs, at least qualitatively.

850-1600 cm^{-1} region. Starting from A(3)-GDYNR and Z(2)-GDYNR, we clearly identify three bands: the first is very close to the G line of 2D-GDY (at 1571 cm^{-1}), the second to the D band (at 1490 cm^{-1}), and the third to the B band (at 983 cm^{-1}). Several satellite lines also show up, giving rise to a rather rich spectrum. This feature is ascribed to the presence of CH bonds on the edges of the ribbons, whose characteristic bending frequencies lie in this spectral region.

By analyzing the vibrational eigenvectors of A(*n*)-GDYNRs, we observe that the band at about 1570 cm^{-1} corresponds to the G mode vibration (ring stretching) of the "bulk" regions, whereas the band at about 1630 cm^{-1} is assigned to the same vibrational pattern, well localized on the edges and coupled to CH wagging vibration. A similar situation is found for the two lines at 1452 and 1499 cm^{-1} : the latter corresponds to the D line of 2D-GDY, and is associated to a "bulk" normal mode, whereas the former shows the same vibrational pattern, mainly localized on peripheral rings and coupled with CH wagging vibrations. Therefore, the lines at 1452 and 1630 cm^{-1} can be taken as markers of armchair edges and, as expected, their relative intensity decreases with increasing the nanoribbon width *n*. These lines are rather intense and should allow a reliable identification of A(*n*)-GDYNRs. Remarkably, thanks to its A_{1g} symmetry, the 1630 cm^{-1} line shows a sizeable Raman intensity also for the largest A(*n*)-GDYNR here investigated (*n* = 5).

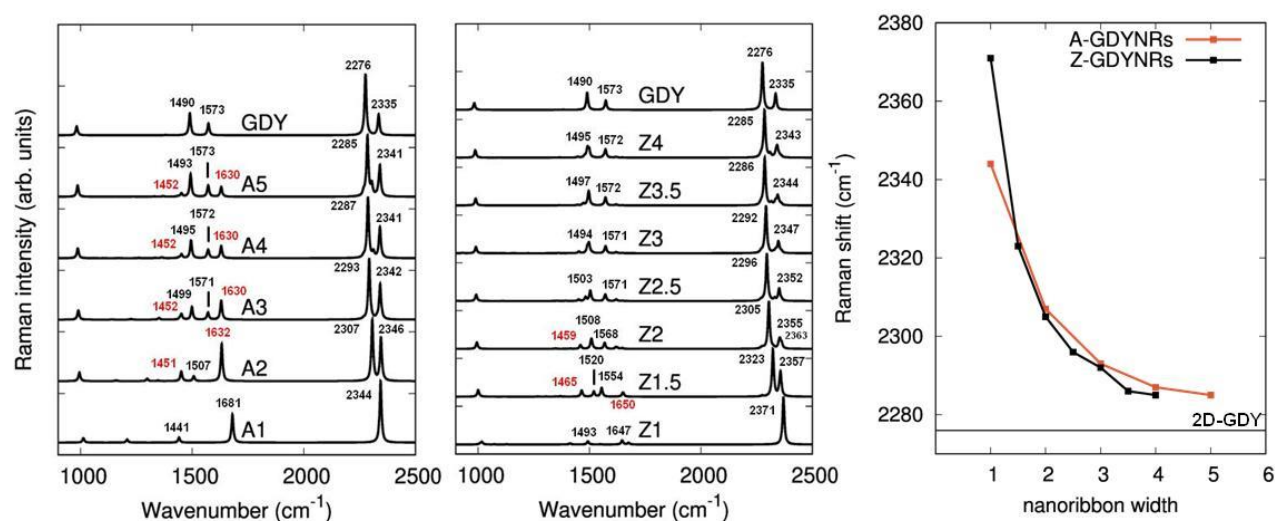


Figure 5: Comparison among the DFT computed (PBE0/6-31G(d)) Raman spectra of 2D-GDY, A(*n*)-GDYNRs (left) and Z(*n*)-GDYNRs (center) having increasing widths. The wavenumber values are not scaled. (right) Modulation of the DFT computed (PBE0/6-31G(d), unscaled values) wavenumber of the Raman Y bands predicted for armchair and zigzag GDYNRs as a function of their width. The wavenumber computed for 2D-GDY is also reported as a comparison.

Considering Z(*n*)-GDYNRs, the inspection of Figure 5 shows that the edge type significantly affects the shape of the Raman spectrum. In the Raman spectra of the thinner Z(*n*)-GDYNRs we observe two bands (1650 cm^{-1} , 1460 cm^{-1}) that are the counterparts of the satellite bands observed for A(*n*)-GDYNRs. However, these lines are significantly weaker in Z(*n*)- than in A(*n*)-GDYNR, which would make more difficult the recognition of Z(*n*)-GDYNRs based on the Raman pattern.

3.3.2 IR spectra

In Figure 6 we compare the IR spectra of A(*n*)- and Z(*n*)-GDYNRs with the spectra of the 1D infinite polymers (A(1) and Z(1)) and 2D-GDY.

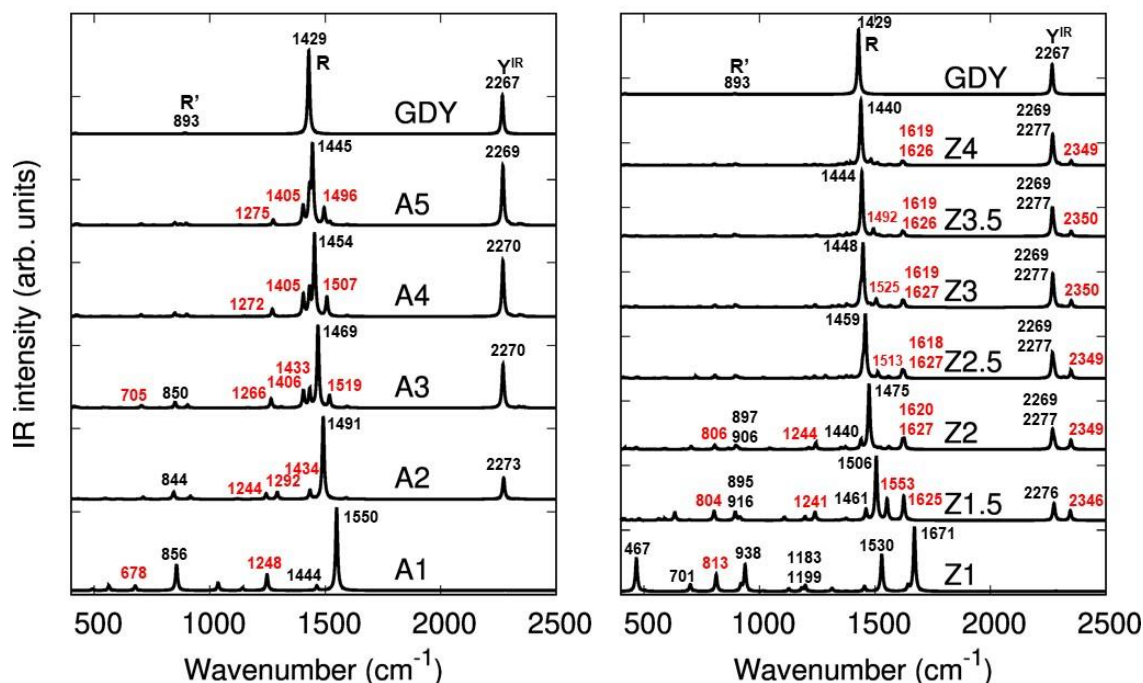


Figure 6: Comparison among the DFT computed (PBE0/6-31G(d)) IR spectra of 2D-GDY, A(*n*)-GDYNRs and Z(*n*)-GDYNRs having increasing widths. The wavenumber values are not scaled.

2000-2500 cm^{-1} region. For both edge types, the polymers A(1) and Z(1) do not show any IR band of appreciable intensity in the sp-carbon region above 2000 cm^{-1} . Starting from A(2) a band raises at about 2270 cm^{-1} , very close to the Y^{IR} band of the 2D crystal. Similarly, in the IR spectrum of Z(*n*)-GDYNRs we find a rather strong Y^{IR} band coming from two close phonons, computed at 2269 and 2277 cm^{-1} . Another IR peak at 2350 cm^{-1} is clearly observed for Z(*n*)-GDYNRs, corresponding to the IR active ECC mode localized on the edges. On the opposite, only a very weak additional absorption band is present for A(*n*)-GDYNRs. This behavior makes this feature a potential marker of Z edges.

850-1600 cm⁻¹ region. The strong R band of 2D-GDY as well as the weak R' find a nice correspondence with two IR features of GYNRs, beginning with A(2) and Z(1.5).

The bands predicted at about 1270 cm⁻¹ and 700 cm⁻¹ in the larger A(*n*)-GDYNRs, even if weak, are significant markers of confinement. While many intense bands are predicted for Z(1), the bands below 1400 cm⁻¹ are weaker in Z(*n*)-GDYNRs: as in the Raman, markers of Z- nanoribbons are difficult to identify, also with IR spectroscopy in this spectral region. A good marker of Z(*n*)-GDYNRs could be the band at about 1620 cm⁻¹, which results from the convolution of two bands computed at 1619 and 1626 cm⁻¹.

In Figures 5 and 6 we highlight in red the more interesting IR and Raman markers of spatial confinement, which are often sensitive to the edge conformation. A brief discussion summarizing the spectroscopic marker bands allowing to distinguish between armchair and zigzag GDYNR is reported in the Supplementary Material [50].

In Supplementary Material [50] we provide also information about Raman tensor properties and dipole derivatives direction of some selected Raman and IR transitions of A(3). These data show that the remarkable ribbon anisotropy determine peculiar polarization properties of the Raman (and IR) transitions, which in turns make suitable the assessment of axial orientation, through polarized Raman and IR experiments.

3.3.3 Effects of the edge groups

In addition to the spectral region above 1000 cm⁻¹, the IR spectra show another frequency range where significant features could be analyzed to discriminate between GDYNR with different edges. In particular, Ref. [45] showed that, similarly to CH stretching modes located in different intramolecular environments [46], also out-of-plane (opla) CH bending normal modes (600-900 cm⁻¹ range) are influenced by the molecular topology. In the case of polycyclic aromatic hydrocarbons (PAHs), out-of-plane CH bending (hereafter referred as opla) modes bring significant information about the edge: indeed, depending on the edge topology different "types" of vibrational patterns, associated to IR transitions, can be identified, each one at characteristic wavenumber. These vibrational patterns are sketched in Figure 7 and are described as collective out of plane displacements of one, two, or three adjacent CH bonds. In the literature, they have been named SOLO, DUO and TRIO [47].

In PAHs, TRIO modes are located at lower wavenumbers than SOLO modes while DUO vibrations are located between these two extremes. Moreover, since these modes are out-of-plane vibrations (orthogonal to the plane of π -conjugated atoms) and are completely localized on terminal CH bonds, they are not affected by π -electron delocalization. Therefore, the same behavior observed in PAHs, should be found also in the case of GDYNR.

We report in Figure 7 the analysis of the 750-950 cm⁻¹ range for 2D-GDY, A(3)- and Z(3)-GDYNR.

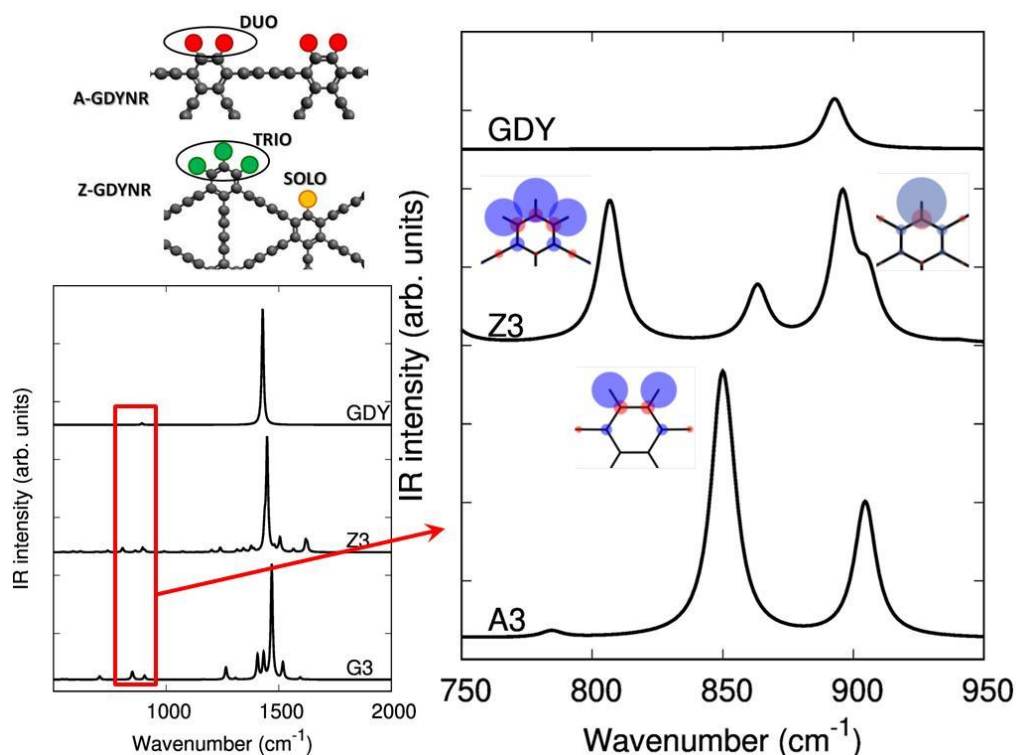


Figure 7: (top, left) Definition of SOLO, DUO and TRIO vibrational patterns associated to opla CH bending normal modes found in A- and Z-GDYNR. (right) Comparison among the DFT computed (PBE0/6-31G(d)) IR spectra of 2D-GDY, with A(3)- and Z(3)-GDYNR in the frequency range 750-950 cm^{-1} where opla CH bending vibrations of the edges are found. Sketched of the OPLA CH normal modes describing the different bands are reported in figure: atomic displacements are indicated by red and purple circles with different colours indicating respectively opposite spatial phases of the motion. The amplitude of the displacement are proportional to the diameter of the circle. The wavenumber values are not scaled.

Even if the opla CH bending vibrations give contributions to the IR spectra weaker than the bands above 1250 cm^{-1} (see the bottom left panel of Figure 7), the bands between 750 and 950 cm^{-1} are non-negligible and are potentially measurable. By analyzing more in details this region, we observe significant differences between A(3)- and Z(3)-GDYNR. A(3)-GDYNR shows two bands at 850 cm^{-1} and 905 cm^{-1} : the latter is reminiscent of a band found in 2D-GDY and it is due to a bulk mode of carbons atoms. As expected, the band at 850 cm^{-1} is an opla CH bending vibration, and it belongs to the DUO pattern. In the case of Z(*n*)-GDYNR, four IR bands are found (807, 863, 896 and 906 cm^{-1}). The bands at 863 cm^{-1} and 896 cm^{-1} are related to bulk modes of carbon domains, while the intense band at 807 cm^{-1} and the shoulder at 906 cm^{-1} are assigned to pure opla CH bending vibrations. In full agreement with the behavior of PAHs, the band at 807 cm^{-1} is associated to TRIO moieties and the band at 906 cm^{-1} to SOLO moieties. Based on these results, we infer that the analysis of IR spectra below 1000 cm^{-1} would allow to detect useful markers able to clearly discriminate A(*n*)-GDYNR from Z(*n*)-GDYNR. We also note that a similar spectroscopic signature is predicted also for Raman-active opla CH bending vibrations. However, their Raman intensity is very weak and probably not measurable.

4. Summary and Conclusion

State-of-the-art periodic boundary conditions DFT calculations have been used here to compute the

band gap and the vibrational response of 2D γ -GDY and related nanoribbons with different widths and edge-type.

We have obtained the following results:

1. The band gap of 2D-GDY (γ -GDY) computed at HSE06/6-31G(d) level of theory (hybrid functional, Gaussian basis set) provides a reliable band gap (1.11 eV), in very good agreement with the value of 1.1 eV obtained by using the GW method.
2. The trends of the band gap as a function of the GDYNRs width, for both armchair (A) and zigzag (Z) edge can be rationalized based on the different structures, and comply with the band gaps of the polymers A(1)-GDYNR and Z(1)-GDYNR, taken as the $n = 1$ width limit.
3. Raman and IR spectra of 2D-GDY have been computed, assigned and discussed in detail, showing a good agreement with available literature data. These spectra can be taken as a reference for the investigation of confined systems and for the interpretation of experimental measurements. Indeed, in a recent work [48], Raman spectroscopy has been applied to characterize GDY grown on graphene, obtaining a nice agreement with previous calculations [27].
4. We have computed the Raman and IR spectra of GDYNRs with different width and edge. We have unveiled Raman markers of A(n)-GDYNR at 1630 cm^{-1} and 1450 cm^{-1} , whereas the weak bands computed at 700 , 1270 and 1405 cm^{-1} are IR markers. In the case of Z(n)-GDYNRs, Raman markers are too weak to be of experimental interest, while the most significant markers are found in the IR spectrum at about 1620 and 2350 cm^{-1} . The Raman bands above 2200 cm^{-1} display an evident redshift for increasing GDYNRs width; hence their position can be useful for a qualitative assessment of the GDYNR width. Apart from minor details, no significant difference has been found in the spectroscopic response of integer vs. half-integer Z(n)-GDYNRs. Finally, IR-active CH out-of-plane modes have been found to have a characteristic dependence on the edge type, providing another significant marker for the characterization of GDYNR.

Our results are relevant as reference spectra of confined GDY-systems, suggesting that both Raman and IR techniques are useful tools for the identification of nanoribbons or to check for the existence of confinement phenomena in 2D-GDY. Our results indicate that it is possible to discriminate systems having different edges, suggesting the application of vibrational spectroscopy for the characterization of topology. As an example in this context, in a very recent paper [49], a combined experimental and computational approach has been used to characterize A1 polymer synthesised on Au surface, providing an interpretation of the bonding processes occurring in the synthesis.

Acknowledgements

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[50] See Supplementary Material at [URL] for : appendix with tables of internal, group and symmetry coordinates of GDY, primitive cell parameters and fractional coordinates of the investigated structures, tables with band gap and vibrational frequencies, IR intensities and Raman activities of the systems and sketches of the normal modes of vibration, marker bands analysis of the investigated systems. Tables with Raman polarizability tensors and dipole moment derivatives of 2D GDY and A3-GDYNR

Supplementary Material:

Raman and IR spectra of graphdiyne nanoribbons

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Appendix

Table A.1: Definition of the internal CC stretching coordinates of 2D-GDY fragments:

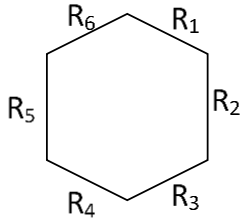
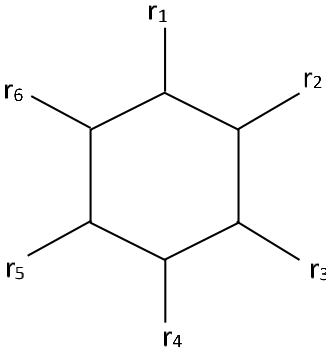
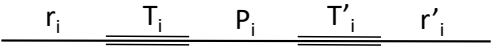
		
CC stretching coordinates $\{R_i\}$ of the aromatic ring	CC stretching $\{r_i\}$ of the polyynic arms. $\{T_i\}$ and $\{P_i\}$ coordinates are defined consistently.	CC stretching coordinates of an individual i -th polyynic arm

Table A.2: Group coordinates of the individual *i*-th polyne arm

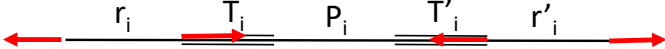
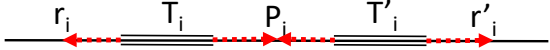
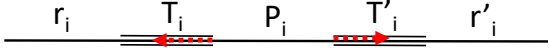
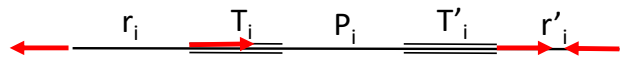
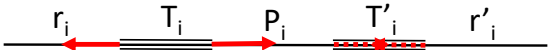
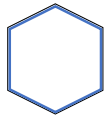
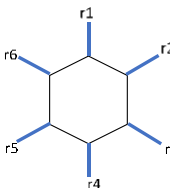
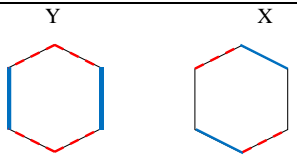
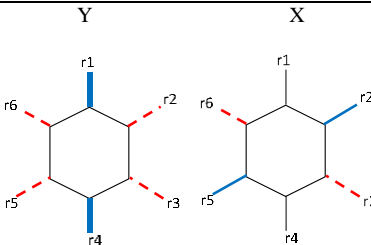
$r_i^+ = \frac{1}{\sqrt{2}} (r_i + r'_i)$	
$T_i^+ = \frac{1}{\sqrt{2}} (T_i + T'_i)$	
P_i	
$r_i^- = \frac{1}{\sqrt{2}} (r_i - r'_i)$	
$T_i^- = \frac{1}{\sqrt{2}} (T_i - T'_i)$	

Table A.3: CC stretching symmetry coordinates of 2D-GDY crystal. Last column: sketch of the stretching pattern associated to each individual symmetry coordinate; bonds which stretch: blue solid line, bonds which shrink: red, broken line.

Symmetry Species	Basis of internal coordinates of the unit cell (ring and polyyne arm)	Basis of group coordinates of six individual polyyne arms	stretching pattern
A_{1g}	$A_{1g}^R = \frac{1}{\sqrt{6}}(R_1 + R_2 + R_3 + R_4 + R_5 + R_6)$		
	$A_{1g}^r = \frac{1}{\sqrt{6}}(r_1 + r_2 + r_3 + r_4 + r_5 + r_6)$	$A_{1g}^{r+} = \frac{1}{\sqrt{6}}(r_1^+ + r_2^+ + r_3^+ + r_4^+ + r_5^+ + r_6^+)$	
	$A_{1g}^T = \frac{1}{\sqrt{6}}(T_1 + T_2 + T_3 + T_4 + T_5 + T_6)$	$A_{1g}^{T+} = \frac{1}{\sqrt{6}}(T_1^+ + T_2^+ + T_3^+ + T_4^+ + T_5^+ + T_6^+)$	the pattern can be deduced considering that of A_{1g}^r
	$A_{1g}^P = \frac{1}{\sqrt{3}}(P_1 + P_2 + P_6)$	$A_{1g}^P = \frac{1}{\sqrt{3}}(P_1 + P_2 + P_3 + P_4 + P_5 + P_6)$	the pattern can be deduced considering that of A_{1g}^r
E_{2g}	$E_{2g}^R(Y) = \frac{1}{\sqrt{12}}(2R_2 + 2R_5 - R_1 - R_3 - R_4 - R_6)$ $E_{2g}^R(X) = \frac{1}{2}(R_1 - R_3 + R_4 - R_6)$		
	$E_{2g}^r(Y) = \frac{1}{\sqrt{12}}(2r_1 + 2r_4 - r_2 - r_3 - r_5 - r_6)$ $E_{2g}^r(X) = \frac{1}{2}(r_2 - r_3 + r_5 - r_6)$	$E_{2g}^{r+}(Y) = \frac{1}{\sqrt{12}}(2r_1^+ + 2r_4^+ - r_2^+ - r_3^+ - r_5^+ - r_6^+)$ $E_{2g}^{r+}(X) = \frac{1}{2}(r_2^+ - r_3^+ + r_5^+ - r_6^+)$	
	$E_{2g}^T(Y) = \frac{1}{\sqrt{12}}(2T_1 + 2T_4 - T_2 - T_3 - T_5 - T_6)$ $E_{2g}^T(X) = \frac{1}{2}(T_2 - T_3 + T_5 - T_6)$	$E_{2g}^{T+}(Y) = \frac{1}{\sqrt{12}}(2T_1^+ + 2T_4^+ - T_2^+ - T_3^+ - T_5^+ - T_6^+)$ $E_{2g}^{T+}(X) = \frac{1}{2}(T_2^+ - T_3^+ + T_5^+ - T_6^+)$	the pattern can be deduced considering that of E_{2g}^r

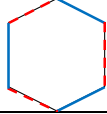
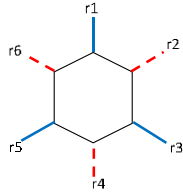
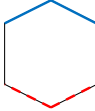
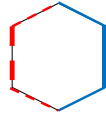
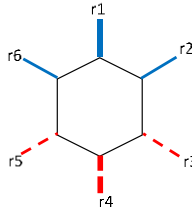
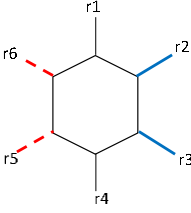
	$E_{2g}^P(Y) = \frac{1}{\sqrt{6}}(2P_1 - P_2 - T_6)$ $E_{2g}^P(X) = \frac{1}{2}(P_2 - P_6)$	$E_{2g}^P(Y) = \frac{1}{\sqrt{12}}(2P_1 + 2P_4 - P_2 - P_3 - P_5 - P_6)$ $E_{2g}^P(X) = \frac{1}{2}(P_2 - P_3 + P_5 - P_6)$	the pattern can be deduced considering that of E_{2g}^r
B_{2u}	$B_{2u}^R = \frac{1}{\sqrt{6}}(R_1 - R_2 + R_3 - R_4 + R_5 - R_6)$		
	$B_{2u}^r = \frac{1}{\sqrt{6}}(r_1 - r_2 + r_3 - r_4 + r_5 - r_6)$	$B_{2u}^{r-} = \frac{1}{\sqrt{6}}(r_1^- - r_2^- + r_3^- - r_4^- + r_5^- - r_6^-)$	
	$B_{2u}^T = \frac{1}{\sqrt{6}}(T_1 - T_2 + T_3 - T_4 + T_5 - T_6)$	$B_{2u}^{T-} = \frac{1}{\sqrt{6}}(T_1^- - T_2^- + T_3^- - T_4^- + T_5^- - T_6^-)$	the pattern can be deduced considering that of B_{2u}^r
E_{1u}	$E_{1u}^R(Y) = \frac{1}{2}(R_1 - R_3 - R_4 + R_6)$ $E_{1u}^R(X) = \frac{1}{\sqrt{12}}(2R_2 - 2R_5 + R_1 + R_3 - R_4 - R_6)$		<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p>Y</p>  </div> <div style="text-align: center;"> <p>X</p>  </div> </div>
	$E_{1u}^r(Y) = \frac{1}{\sqrt{12}}(2r_1 - 2r_4 + r_2 - r_3 - r_5 + r_6)$ $E_{1u}^r(X) = \frac{1}{2}(r_2 + r_3 - r_5 - r_6)$	$E_{1u}^{r-}(Y) = \frac{1}{\sqrt{12}}(2r_1^- - 2r_4^- + r_2^- - r_3^- - r_5^- + r_6^-)$ $E_{1u}^{r-}(X) = \frac{1}{2}(r_2^- + r_3^- - r_5^- - r_6^-)$	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;"> <p>Y</p>  </div> <div style="text-align: center;"> <p>X</p>  </div> </div>
	$E_{1u}^T(Y) = \frac{1}{\sqrt{12}}(2T_1 - 2T_4 + T_2 - T_3 - T_5 + T_6)$ $E_{1u}^T(X) = \frac{1}{2}(T_2 + T_3 - T_5 - T_6)$	$E_{1u}^{T-}(Y) = \frac{1}{\sqrt{12}}(2T_1^- - 2T_4^- + T_2^- - T_3^- - T_5^- + T_6^-)$ $E_{1u}^{T-}(X) = \frac{1}{2}(T_2^- + T_3^- - T_5^- - T_6^-)$	the pattern can be deduced considering that of E_{1u}^r

Table S1: DFT computed [PBE0/6-31G(d)] primitive cell parameters (in Angstrom) and fractional coordinates of 2D-GDY

space group :P 6/MMM

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.44081102	9.44081102	500.00000000	90.000000	90.000000	120.000000

ATOMS IN THE ASYMMETRIC UNIT 3 - ATOMS IN THE UNIT CELL: 18

ATOM	X/A	Y/B	Z(ANGSTROM)
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C	0.000000000000E+00	1.502058239380E-01	0.000000000000E+00
C	0.000000000000E+00	-1.502058239380E-01	0.000000000000E+00
C	-1.502058239380E-01	-1.502058239380E-01	0.000000000000E+00
C	1.502058239380E-01	1.387778780781E-17	0.000000000000E+00
C	-1.502058239380E-01	-1.387778780781E-17	0.000000000000E+00
C	1.502058239380E-01	1.502058239380E-01	0.000000000000E+00
C	-2.991003876810E-01	-2.775557561563E-17	0.000000000000E+00
C	2.991003876810E-01	2.775557561563E-17	0.000000000000E+00
C	-2.721815550437E-17	-2.991003876810E-01	0.000000000000E+00
C	2.991003876810E-01	2.991003876810E-01	0.000000000000E+00
C	-2.991003876810E-01	-2.991003876810E-01	0.000000000000E+00
C	2.721815550437E-17	2.991003876810E-01	0.000000000000E+00
C	-4.284415967800E-01	0.000000000000E+00	0.000000000000E+00
C	4.284415967800E-01	2.775557561563E-17	0.000000000000E+00
C	0.000000000000E+00	-4.284415967800E-01	0.000000000000E+00
C	4.284415967800E-01	4.284415967800E-01	0.000000000000E+00
C	-4.284415967800E-01	-4.284415967800E-01	0.000000000000E+00
C	0.000000000000E+00	4.284415967800E-01	0.000000000000E+00

Table S2: DFT computed [PBE0/6-31G(d)] primitive cell parameters and fractional coordinates of A(n)-GDYNR of different widths. Space groups are all P1.

A1

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.43619694	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 14 - ATOMS IN THE UNIT CELL: 14

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	2.212034929497E-01	1.211539588444E+00	2.654137930430E-04
C	7.475810552195E-02	1.211716427417E+00	2.994996334514E-04
C	-4.238964086493E-01	3.698240912281E-06	-1.026613190419E-06
C	-2.801454905482E-01	4.872875894212E-06	2.999029709488E-06
C	4.467980866812E-01	-1.098926222355E-04	3.219440647709E-06
C	-1.508389950894E-01	8.677619826011E-05	-1.204768866295E-05
C	2.968774159284E-01	-6.511564883681E-05	6.230821559945E-05
C	-9.331936697957E-04	3.509700334213E-05	-4.328741689435E-05
H	2.793218922936E-01	2.148492927733E+00	3.932939710312E-04
C	2.211942712962E-01	-1.211616314353E+00	-2.611670848359E-04
C	7.474883748800E-02	-1.211696375321E+00	-3.405211587565E-04
H	1.668152338480E-02	2.148848961456E+00	5.262876417629E-04
H	2.793052858649E-01	-2.148610565712E+00	-6.032846907945E-04
H	1.666517654799E-02	-2.148790085712E+00	-5.616870721088E-04

A2

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.43869055	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 32 - ATOMS IN THE UNIT CELL: 32

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	-4.254000625681E-01	9.399187332857E+00	3.086078600736E-04
C	-2.791343574068E-01	9.399124893117E+00	-5.806113996774E-04
H	-4.835436994160E-01	1.033551288806E+01	5.209927012823E-04
C	4.981486340743E-01	8.193882978524E+00	3.840369790689E-04
H	-2.209808604232E-01	1.033539924091E+01	-1.208455334460E-03
C	-2.026834746840E-01	8.193803890603E+00	-1.130373674865E-04
C	-5.329187136983E-02	8.206608854863E+00	5.236628716020E-05
C	-4.273942038309E-01	6.960837973132E+00	5.766815097722E-04
C	7.600739486134E-02	8.224823455280E+00	-2.014476441927E-04
C	-2.771448082145E-01	6.960725877736E+00	7.011788936198E-04
C	2.194547002114E-01	8.224888730501E+00	-2.181637874389E-04
C	4.981534321064E-01	5.740238384991E+00	3.163516372525E-05
C	3.487554169970E-01	8.206645568051E+00	-1.048552930959E-05
C	4.336187951974E-01	4.682818528881E+00	-7.459053912106E-04

C -2.026875999680E-01 5.740183280177E+00 8.058154158979E-04
 C 3.622452177501E-01 3.509764208636E+00 -1.390054891331E-03
 C -1.378564439804E-01 4.684354044254E+00 7.602666949035E-04
 C 2.977135061582E-01 2.452324431623E+00 -1.849872725450E-03
 C 7.280333371417E-02 1.234865263202E+00 -8.595345136725E-04
 C 2.230466825579E-01 1.232924030973E+00 -5.463181059646E-04
 C -6.631891509260E-02 3.512168941979E+00 2.623627782419E-04
 C -1.836669748748E-03 2.754171089640E-03 2.833479256309E-06
 C -1.495102010349E-03 2.456330180625E+00 -8.681242652421E-04
 C 2.973314492072E-01 -1.161951415020E-03 -5.465493040682E-04
 C 7.443823853555E-02 -1.203545543557E+00 5.440960388187E-04
 C 4.467219094107E-01 -1.556155531468E-02 -5.667888299237E-04
 C -4.239741768687E-01 -3.034562941349E-02 -4.603384317417E-04
 C 2.207079709870E-01 -1.205450337767E+00 6.702874792862E-04
 C -2.805332216125E-01 -2.911924648773E-02 -3.005250356739E-04
 C -1.512359788744E-01 -8.589842401511E-03 -1.788584233349E-04
 H 1.614628446324E-02 -2.139042191055E+00 2.548893861617E-03
 H 2.787144798369E-01 -2.142530852650E+00 1.435015837465E-03

A3

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.43907321	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 50 - ATOMS IN THE UNIT CELL: 50

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C -9.308873694425E-03 -2.138885297421E-01 2.347323029239E-02
 C 6.707350216770E-02 9.220923777800E-01 -3.807778986710E-01
 H 8.830412508931E-03 1.803520912578E+00 -6.947773462818E-01
 C 6.524974064744E-02 -1.375135543327E+00 4.371699278943E-01
 C 2.133363900703E-01 9.232987004311E-01 -3.809330346334E-01
 C 2.155328689350E-01 -1.373595702395E+00 4.374257598518E-01
 C 2.899021532066E-01 -2.113489879464E-01 2.379006871945E-02
 C 2.901874291557E-01 -2.521496984476E+00 8.475642639247E-01
 H 2.714076528965E-01 1.805617519551E+00 -6.952764871588E-01
 C 3.542329348589E-01 -3.521264120074E+00 1.200594758137E+00
 C 4.392850659142E-01 -1.986275973606E-01 1.942352171978E-02
 C 4.257120922383E-01 -4.625956521381E+00 1.590926399576E+00
 C 4.903123579543E-01 -5.622151746090E+00 1.945821174540E+00
 C 4.900432897069E-01 -7.923596726907E+00 2.771802573315E+00
 C -4.314119122596E-01 -1.849210546814E-01 1.464828609016E-02
 C -4.350139928959E-01 -6.770434362813E+00 2.347734591007E+00
 C -4.348117269065E-01 -9.082738328042E+00 3.175546974587E+00
 C -2.879871636280E-01 -1.856874291296E-01 1.458466969749E-02
 C -2.848482098441E-01 -6.765453655889E+00 2.357302301283E+00
 C -2.846425446667E-01 -9.078068432344E+00 3.184515770735E+00
 C -2.096981123467E-01 -7.925129817965E+00 2.759952170664E+00
 C -2.104967038589E-01 -5.619956846324E+00 1.941486852952E+00

C	-1.586887649373E-01	-2.022137869098E-01	1.969130297656E-02
C	-1.459130178620E-01	-4.622589848485E+00	1.589285804665E+00
C	-7.429619006216E-02	-3.519545065958E+00	1.196476845704E+00
C	-9.190339085525E-03	-2.525330031181E+00	8.446982249289E-01
C	-6.075871298043E-02	-7.922221943237E+00	2.766462052915E+00
C	6.859666314635E-02	-7.924788502257E+00	2.765358174276E+00
C	2.117578550339E-01	-7.924880211134E+00	2.767685930058E+00
C	3.411055282175E-01	-7.926814375336E+00	2.765517002088E+00
C	2.132736064664E-01	-1.675505057153E+01	5.957473066003E+00
C	6.700758282943E-02	-1.675548171351E+01	5.957080169885E+00
C	-4.315846827399E-01	-1.565008626736E+01	5.555608401119E+00
C	4.391128219107E-01	-1.563414418134E+01	5.550684727187E+00
C	2.897333553649E-01	-1.562198151480E+01	5.546452730888E+00
C	-9.486989067326E-03	-1.562294534157E+01	5.545180274041E+00
C	-1.588604511563E-01	-1.563523531786E+01	5.549206678379E+00
C	-2.881592468555E-01	-1.565060806887E+01	5.555170680436E+00
C	2.152409619868E-01	-1.446293047724E+01	5.125834028228E+00
C	6.497238603948E-02	-1.446370472169E+01	5.124548137080E+00
C	2.897156659801E-01	-1.331557833370E+01	4.711133216055E+00
C	-9.526563082916E-03	-1.331767630971E+01	4.706703906784E+00
C	4.908573565516E-01	-1.022684812709E+01	3.594936502467E+00
C	4.262016025559E-01	-1.122186533010E+01	3.952455630617E+00
C	3.545966710407E-01	-1.232262875885E+01	4.352136904728E+00
C	-7.465834821595E-02	-1.232729256736E+01	4.344724439197E+00
C	-2.101462970937E-01	-1.022674153893E+01	3.588634212943E+00
C	-1.460049112593E-01	-1.122384745535E+01	3.948569891348E+00
H	2.714479643607E-01	-1.763498059038E+01	6.276798031921E+00
H	8.866842754113E-03	-1.763551617170E+01	6.276714504841E+00

A4

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.43895056	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 68 - ATOMS IN THE UNIT CELL: 68

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	-4.484364735474E-01	2.470859598131E+01	8.297619404729E+00
C	-3.021656616272E-01	2.470843741747E+01	8.295715057842E+00
C	4.750297456446E-01	2.356840643126E+01	7.907976348164E+00
H	4.934663617475E-01	2.559428592243E+01	8.602176107584E+00
C	-2.257509196278E-01	2.356763228916E+01	7.905707280242E+00
H	-2.439411620731E-01	2.559395325959E+01	8.599187548842E+00
C	-4.505588714091E-01	2.240118846507E+01	7.509352835262E+00
C	-7.638025890143E-02	2.358005022719E+01	7.908131419933E+00
C	5.292181772888E-02	2.359630147145E+01	7.914285220079E+00
C	-3.002842864729E-01	2.240073618467E+01	7.507954664397E+00
C	4.748470373729E-01	2.124737034878E+01	7.115022350690E+00
C	1.963634279144E-01	2.359648253321E+01	7.914545443523E+00

C 3.256657367142E-01 2.358025930202E+01 7.913515424629E+00
C 4.103049669101E-01 2.024658303232E+01 6.772539787053E+00
C -2.258249870878E-01 2.124570407140E+01 7.114833746931E+00
C 3.389045949142E-01 1.913632276259E+01 6.396297732764E+00
C -1.607775014441E-01 2.024705833869E+01 6.774571505947E+00
C 2.747257401165E-01 1.813326669890E+01 6.053967490601E+00
C 4.974890848640E-02 1.698288998852E+01 5.666134301903E+00
C 1.999208340237E-01 1.697756748058E+01 5.676262941951E+00
C -8.915558290775E-02 1.913865617223E+01 6.396802372293E+00
C -2.549919336085E-02 1.581490289845E+01 5.289746961894E+00
C 2.748041614867E-01 1.581589526572E+01 5.274837140492E+00
C -2.454328357608E-02 1.813608246869E+01 6.060733796806E+00
C 4.937690600232E-02 1.465260900775E+01 4.889831699020E+00
C 4.237260738798E-01 1.581197498828E+01 5.281024387169E+00
C 1.995787925273E-01 1.464770662130E+01 4.899003682859E+00
C -4.469197203688E-01 1.581235436947E+01 5.280291107332E+00
C -2.518508075259E-02 1.349457428088E+01 4.516048274063E+00
C -3.037618618827E-01 1.581222203651E+01 5.283466700918E+00
C -1.744165630581E-01 1.581883687897E+01 5.283676652467E+00
C -8.977233760057E-02 1.249063374101E+01 4.182566661155E+00
C 2.739998286621E-01 1.349522153559E+01 4.506146189623E+00
C -1.612042505683E-01 1.137891527727E+01 3.814227824395E+00
C 3.391716645953E-01 1.249323019995E+01 4.176814152130E+00
C -2.252809929348E-01 1.037148307722E+01 3.482462720408E+00
C 4.109345613987E-01 1.138295720063E+01 3.810615859188E+00
C -4.502946640378E-01 9.217958339882E+00 3.106808938049E+00
C -3.000969697079E-01 9.219250685693E+00 3.095366786582E+00
C 4.744672900287E-01 8.055714733304E+00 2.712940661926E+00
C 4.753860804868E-01 1.037821181675E+01 3.477715015348E+00
C -2.252649108694E-01 8.047722400987E+00 2.722465315649E+00
C -7.634191067815E-02 8.048456172690E+00 2.714591246939E+00
C -4.506977321380E-01 6.884278037317E+00 2.340179499713E+00
C 5.301574389113E-02 8.051236669514E+00 2.717386931859E+00
C -3.005088953854E-01 6.885589745106E+00 2.328482399057E+00
C 1.962000069899E-01 8.053306410806E+00 2.716374567980E+00
C 3.255480833876E-01 8.055092103668E+00 2.720854962018E+00
C 4.745514239980E-01 5.731687486445E+00 1.952307865487E+00
C 4.104641955405E-01 4.724301897882E+00 1.621514990213E+00
C -2.261696604982E-01 5.725725504116E+00 1.955268382939E+00
C 3.389107053476E-01 3.612625176588E+00 1.252180236870E+00
C -1.615941667197E-01 4.721725293732E+00 1.622291349969E+00
C 2.745627711318E-01 2.607681146776E+00 9.188984497201E-01
C 4.956908032118E-02 1.450159914016E+00 5.408347319320E-01
C 1.998406637000E-01 1.449676457653E+00 5.394173873673E-01
C -8.986534113233E-02 3.609920590621E+00 1.256499390716E+00
C -2.495220532232E-02 2.792518751962E-01 1.546691269886E-01
C -2.494381248401E-02 2.607713904875E+00 9.251952887632E-01
C 2.742433431660E-01 2.783364312804E-01 1.525987029070E-01
C 5.145503976708E-02 -8.653821227322E-01 -2.238321906383E-01

C	4.236208966743E-01	2.659304066495E-01	1.486440680759E-01
C	1.977236364824E-01	-8.660855292267E-01	-2.243275561409E-01
C	-4.470716957205E-01	2.507888209554E-01	1.440544578392E-01
C	-3.036289637902E-01	2.513714565911E-01	1.449369686345E-01
C	-1.743278013714E-01	2.671660693677E-01	1.503716018368E-01
H	-6.760630950148E-03	-1.753964230564E+00	-5.175109545170E-01
H	2.558232289683E-01	-1.755305892457E+00	-5.180914193576E-01

A5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
9.43958534	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 86 - ATOMS IN THE UNIT CELL: 86

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
C	-7.295725578702E-03	-1.374838629765E+01	9.544323903213E+00
C	6.774280145206E-02	-1.274010423489E+01	8.842667219211E+00
C	6.782092039848E-02	-1.474186880218E+01	1.026602828210E+01
C	2.179479303095E-01	-1.274500162108E+01	8.835123506379E+00
C	2.180359264253E-01	-1.474695136589E+01	1.025818192688E+01
C	2.930687131090E-01	-1.373882801699E+01	9.556322985811E+00
C	2.925183538835E-01	-1.573232908345E+01	1.097252029512E+01
C	3.568989372267E-01	-1.659458972305E+01	1.158730099929E+01
C	4.419726907302E-01	-1.374288547151E+01	9.549754723029E+00
C	4.284357301733E-01	-1.754645125003E+01	1.226825591209E+01
C	4.932266265634E-01	-1.840569785678E+01	1.288352192512E+01
C	-4.286719072086E-01	-1.374164949944E+01	9.551035572010E+00
C	4.927123152279E-01	-2.039001815138E+01	1.431193366477E+01
C	-4.322279749057E-01	-1.940012138507E+01	1.358496257135E+01
C	-4.322100584286E-01	-2.139289738749E+01	1.502049194357E+01
C	-2.855526861424E-01	-1.374369690106E+01	9.548550893754E+00
C	-2.820336872096E-01	-1.939465388064E+01	1.359230691734E+01
C	-2.075449578228E-01	-1.841157617184E+01	1.287443091592E+01
C	-2.820227091130E-01	-2.138672071931E+01	1.502895924039E+01
C	-1.425789122063E-01	-1.755239408934E+01	1.226074990503E+01
C	-2.069512168978E-01	-2.039800550970E+01	1.430055710596E+01
C	-1.561979275332E-01	-1.374428000071E+01	9.550851404837E+00
C	-7.099613033653E-02	-1.660041709425E+01	1.158038552276E+01
C	-6.592275316372E-03	-1.573920309494E+01	1.096428783871E+01
C	2.160737139085E-01	-2.800730484494E+01	1.980039620678E+01
C	2.179316036323E-01	-2.602911978172E+01	1.837526140514E+01
C	2.924918775214E-01	-2.702889228276E+01	1.909631298731E+01
C	-7.149518264378E-02	-2.418550626165E+01	1.704084579641E+01
C	-6.749351189528E-03	-2.703132976096E+01	1.909594209483E+01
C	-1.430404418425E-01	-2.323483683033E+01	1.635692799552E+01
C	-2.076464337297E-01	-2.237852460406E+01	1.573631125224E+01
C	6.981120798358E-02	-2.800826372998E+01	1.980061805150E+01
C	-6.945376906231E-03	-2.504250661965E+01	1.766067736451E+01

C 6.766957912949E-02 -2.603065051043E+01 1.837480336082E+01
H 1.176673585286E-02 -2.876863128749E+01 2.034766363074E+01
H 2.742420841851E-01 -2.876656073638E+01 2.034769635911E+01
C -5.803674042584E-02 -2.039351550886E+01 1.430612310040E+01
C 7.130471934786E-02 -2.039175539445E+01 1.430273711954E+01
C 2.144558706611E-01 -2.038997677112E+01 1.430482912206E+01
C 3.437943687077E-01 -2.039427338946E+01 1.430579582130E+01
C 6.975390379720E-02 6.078645914188E-01 -5.776139724315E-01
C -6.791977434202E-03 -3.772126565336E-01 1.159795579925E-01
C 2.160160691009E-01 6.073445472807E-01 -5.771976171294E-01
C 6.764554355039E-02 -1.385493040932E+00 8.261129021906E-01
C 2.924525533469E-01 -3.779984628636E-01 1.170726268300E-01
C 2.179082691485E-01 -1.385638016764E+00 8.270893572832E-01
C 4.418214159207E-01 -3.676178513971E-01 1.102161173043E-01
C 2.922849724473E-01 -2.382181794217E+00 1.531631873602E+00
C -4.288833033348E-01 -3.544083099983E-01 1.002623360507E-01
C -2.854592865116E-01 -3.541906875206E-01 9.963899549480E-02
C 3.566409770910E-01 -3.247756528667E+00 2.141234617078E+00
C -1.561613749000E-01 -3.668216760370E-01 1.081396271452E-01
C 4.283484258693E-01 -4.206019136313E+00 2.813208326865E+00
C -7.161559554360E-02 -3.247504909457E+00 2.135398729171E+00
C -6.855219496566E-03 -2.383391959843E+00 1.527512209263E+00
C -1.430988268731E-01 -4.204555313400E+00 2.811086651311E+00
C 4.933441173836E-01 -5.067889333687E+00 3.422286632533E+00
C -2.076517469392E-01 -5.070229624155E+00 3.418935448759E+00
C 2.923431110400E-01 -1.174609767945E+01 8.138988310420E+00
H 1.169150596208E-02 1.373662578840E+00 -1.116925270364E+00
C -2.820600099683E-01 -6.061162517371E+00 4.127008864673E+00
C -4.322426971903E-01 -6.067491207402E+00 4.118090516362E+00
C 3.570574044670E-01 -1.088389542864E+01 7.527239528333E+00
C -2.069646105140E-01 -7.072245491630E+00 4.823705771098E+00
C -5.805387430369E-02 -7.068039258846E+00 4.829521479687E+00
C 4.927021047116E-01 -7.064229750920E+00 4.835592789044E+00
C 4.286363808259E-01 -9.928302362870E+00 6.851829729144E+00
C -6.708716457986E-03 -1.175313742479E+01 8.130255846506E+00
C 7.128679149440E-02 -7.070215115552E+00 4.828576691998E+00
H 2.741772515427E-01 1.372729580224E+00 -1.116172916944E+00
C 4.932940701673E-01 -9.063679365332E+00 6.242942597411E+00
C -2.820168019551E-01 -8.069643084407E+00 5.540430525947E+00
C 2.144473933397E-01 -7.068698971205E+00 4.831114870667E+00
C -7.097259378676E-02 -1.088814822106E+01 7.518222966508E+00
C -4.322055963874E-01 -8.074826159222E+00 5.533179780027E+00
C 3.437900596335E-01 -7.068981863311E+00 4.829791107234E+00
C -2.074828611532E-01 -9.070688855271E+00 6.232559684734E+00
C -1.425064529631E-01 -9.932649892057E+00 6.842183860541E+00
C 4.933842242019E-01 -2.237589603852E+01 1.573969583511E+01
C 4.288651445585E-01 -2.323430561599E+01 1.635815572929E+01
C 3.573429903166E-01 -2.418280315126E+01 1.704545841028E+01
C 2.923294875578E-01 -2.503873610716E+01 1.766235376713E+01

C	-1.561117135474E-01	-2.704190282219E+01	1.910368845597E+01
C	-2.854133898984E-01	-2.705343396447E+01	1.911212460482E+01
C	-4.288387625300E-01	-2.705261958900E+01	1.911232751782E+01
C	4.418652332222E-01	-2.703896613516E+01	1.910335768437E+01

Table S3: DFT computed [PBE0/6-31G(d)] primitive cell parameters and fractional coordinates of Z(n)-GDYNR of different widths. Space groups are all P1

Z1

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.36146819	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 28 - ATOMS IN THE UNIT CELL: 28

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	-4.261216250627E-01	-5.308159610809E+00	-1.002590944289E+00
C	-4.998120399951E-01	-4.632289595237E+00	-8.743345226672E-01
C	7.387313789957E-02	-6.841465995049E-01	-1.294678883841E-01
C	-2.767498846060E-01	-2.553898981741E+00	-4.836278158277E-01
C	-4.087093752024E-04	-6.298682417201E-04	-5.166814214113E-04
C	-3.524322197236E-01	-4.632074347445E+00	-8.753091443112E-01
C	-2.121018733674E-01	-1.958678952062E+00	-3.717118574054E-01
C	4.995910801751E-01	-3.251490461605E+00	-6.136834312481E-01
C	-1.401119305652E-01	-1.293676306281E+00	-2.462398797615E-01
C	4.245016627384E-01	-2.554355644389E+00	-4.816311239544E-01
C	3.598512529245E-01	-1.959375438328E+00	-3.689653817318E-01
C	-7.550854260742E-02	-6.973551093066E-01	-1.334457076090E-01
C	2.878602977017E-01	-1.294410121744E+00	-2.432410157531E-01
C	2.232537174692E-01	-6.981835405084E-01	-1.304746312136E-01
C	1.481604172761E-01	-9.610795318600E-04	8.422105198642E-04
C	1.894309412521E-04	1.380020272516E+00	2.610089695694E-01
C	-3.518377880418E-01	-3.251271071488E+00	-6.146520600084E-01
C	-4.261241441948E-01	-2.567961063701E+00	-4.850131459254E-01
C	1.475693743039E-01	1.379670329076E+00	2.626087369791E-01
C	7.387876812351E-02	2.055834025969E+00	3.898647823588E-01
H	-4.261204188858E-01	-6.375760309897E+00	-1.204339570497E+00
H	4.424704759539E-01	-5.158535016393E+00	-9.732004049514E-01
H	7.386955570280E-02	-1.749927068431E+00	-3.316086442809E-01
H	-5.753216936543E-02	1.906140867178E+00	3.600930021159E-01
H	-4.261252272210E-01	-1.502059455135E+00	-2.835913825237E-01
H	2.052889659862E-01	1.905553350019E+00	3.630260726598E-01
H	7.388032249679E-02	3.123384972666E+00	5.919565958751E-01
H	-2.947138866816E-01	-5.158154175642E+00	-9.749451363138E-01

Z1.5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35142899	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 46 - ATOMS IN THE UNIT CELL: 46

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C -7.588331797034E-02 -1.693963654703E+00 1.301173508778E+00
 C -1.400757530615E-01 -2.194492304413E+00 1.670410624436E+00
 C -2.118418349880E-01 -2.739825409022E+00 2.073153543314E+00
 C -2.769135264859E-01 -3.219743944576E+00 2.427236294929E+00
 C -3.533648080872E-01 -4.904532649100E+00 3.674967074809E+00
 C -3.521742045948E-01 -3.778646067269E+00 2.840828164458E+00
 C -4.270209833359E-01 -5.459765076838E+00 4.085319481558E+00
 C -4.270570025783E-01 -3.200654066469E+00 2.412458388890E+00
 C 4.993030346758E-01 -4.905691793665E+00 3.674280941373E+00
 C 4.980760480162E-01 -3.779504668374E+00 2.840599335050E+00
 H 4.415141883786E-01 -5.335134124980E+00 3.991914617876E+00
 C 4.228030625814E-01 -3.220723861238E+00 2.427444350948E+00
 C 3.577739193531E-01 -2.741119332423E+00 2.070859252888E+00
 C 2.859648811424E-01 1.111056357088E+00 -7.730642434166E-01
 C 2.217932288423E-01 6.100692278728E-01 -4.035160727842E-01
 C 3.577180569229E-01 1.656956191177E+00 -1.175545970825E+00
 C -4.270812069571E-01 -2.069171762603E+00 1.574342812464E+00
 C 2.860183557783E-01 -2.195478149176E+00 1.668004301106E+00
 C -4.271148417420E-01 -1.087303258248E+00 8.493240113345E-01
 C 4.227937377978E-01 2.137206544213E+00 -1.528937352270E+00
 C -4.271077454502E-01 1.193512413598E-03 4.600852259454E-02
 C 4.980683972892E-01 2.696850261691E+00 -1.940850477198E+00
 C -4.271089931399E-01 9.834109865640E-01 -6.785378645577E-01
 C 2.218933060030E-01 -1.693678265368E+00 1.297342138707E+00
 C 4.993038807782E-01 3.825386989603E+00 -2.771347510661E+00
 C -4.270721528329E-01 2.116985101940E+00 -1.513835572728E+00
 C 1.475599253187E-01 3.126877013578E-02 2.441928206912E-02
 C -4.270148066535E-01 4.380949116768E+00 -3.180099526243E+00
 C 1.476093160920E-01 -1.115212493657E+00 8.713114050473E-01
 C -3.521835781960E-01 2.696255163229E+00 -1.940192276637E+00
 C -3.533635133806E-01 3.824757944267E+00 -2.770784551522E+00
 C 7.291334159046E-02 5.782894226976E-01 -3.794229601971E-01
 C -2.769313356935E-01 2.136113106056E+00 -1.527889305987E+00
 C -2.118738236051E-01 1.656490011856E+00 -1.172750829780E+00
 C -1.401215279909E-01 1.110543098709E+00 -7.702760679141E-01
 C 7.300594129861E-02 -1.662948736065E+00 1.276454160631E+00
 C -1.690378797442E-03 3.084362248206E-02 2.611593276921E-02
 C -7.596477529902E-02 6.092188517744E-01 -4.004754486681E-01
 C -1.642069727354E-03 -1.115571899147E+00 8.730910113214E-01
 H 4.415185696692E-01 4.255689093280E+00 -3.087983566361E+00
 H 7.287544760975E-02 1.450266128471E+00 -1.024570754706E+00
 H -4.269907722819E-01 5.255680609764E+00 -3.823985980205E+00
 H -2.955559374881E-01 4.254199946893E+00 -3.087487113344E+00
 H 7.304433334054E-02 -2.535546255026E+00 1.920757419223E+00
 H -2.955607996497E-01 -5.332796895551E+00 3.993460803683E+00
 H -4.270052824913E-01 -6.332555391036E+00 4.731826065746E+00

Z2

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35211046	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 64 - ATOMS IN THE UNIT CELL: 64					
ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)		

C	-1.805781448494E-03	6.176159581136E+00	7.296902219224E+00		
C	7.274710565433E-02	6.610830317552E+00	7.822867409737E+00		
C	-2.420509817927E-03	5.272397485956E+00	6.198925520814E+00		
H	7.275661400434E-02	7.300273411948E+00	8.659976338905E+00		
C	1.472865039755E-01	6.177790036660E+00	7.295176565251E+00		
C	2.216014051218E-01	6.635043800467E+00	7.848635984577E+00		
C	7.272318705174E-02	4.824272465493E+00	5.652972643336E+00		
C	2.857327847087E-01	7.031077733265E+00	8.330100765180E+00		
C	1.478756132708E-01	5.273392490451E+00	6.197717729973E+00		
C	3.575081218705E-01	7.459187940227E+00	8.855115022460E+00		
C	7.271599808641E-02	3.928944166995E+00	4.565466998697E+00		
C	4.990663290516E-01	9.164209549521E+00	1.093797634509E+01		
C	4.226073415830E-01	7.835456575180E+00	9.316661439996E+00		
C	7.268345342374E-02	3.153874779802E+00	3.622945027670E+00		
C	2.222481987685E-01	4.825564581559E+00	5.653902710402E+00		
C	-4.272734742712E-01	9.601247932418E+00	1.147220234241E+01		
C	4.978693232807E-01	8.274681191250E+00	9.855327766815E+00		
H	4.412754834800E-01	9.504580739325E+00	1.134937450631E+01		
C	7.265826708552E-02	2.295715914400E+00	2.576915419519E+00		
C	2.869750033947E-01	4.438120666450E+00	5.183874872325E+00		
C	7.264754103096E-02	1.521675773499E+00	1.633290315570E+00		
H	-4.272832071644E-01	1.029109277967E+01	1.231114458321E+01		
C	-3.536007357624E-01	9.162397627633E+00	1.093993418489E+01		
C	-4.272480078313E-01	7.816533301264E+00	9.300697987611E+00		
C	-2.168613965340E-03	1.739838558553E-01	-1.382840663125E-02		
C	-3.523797923698E-01	8.272757715753E+00	9.857391964307E+00		
C	7.268486547239E-02	6.302037943836E-01	5.434031360267E-01		
C	-4.272350670818E-01	6.922238403396E+00	8.213092054235E+00		
C	3.584940416047E-01	4.006772984327E+00	4.661532615467E+00		
C	-9.139764833374E-04	-7.128004615558E-01	-1.098725134182E+00		
C	-4.272354707463E-01	6.146555658688E+00	7.270831530571E+00		
C	4.232102228527E-01	3.619005429232E+00	4.191397950600E+00		
C	-4.272457457975E-01	5.287359936704E+00	6.225755928184E+00		
C	1.475823204512E-01	1.753629722089E-01	-1.335209127113E-02		
C	7.277454515209E-02	-1.148598033793E+00	-1.632930586681E+00		
H	-5.868479580687E-02	-1.051508176683E+00	-1.512281752455E+00		
C	2.228267536426E-01	6.151905530859E-01	5.254302963742E-01		
C	-4.272769460259E-01	4.512574456241E+00	5.283002374970E+00		
C	2.879441942888E-01	9.911001056074E-01	9.865700499793E-01		
C	1.464205797245E-01	-7.114446207969E-01	-1.098232968749E+00		
C	4.975900448831E-01	3.170975598381E+00	3.648060636269E+00		
C	3.597282230454E-01	1.418247546347E+00	1.512233737345E+00		
C	-4.272647566889E-01	3.618758326607E+00	4.194226287295E+00		

C	4.238848910780E-01	1.813183718702E+00	1.993679756249E+00
C	4.981901644927E-01	2.268508891158E+00	2.548996640061E+00
C	-3.521171386627E-01	3.170425693024E+00	3.648597312074E+00
C	-4.272640064579E-01	1.835142894132E+00	2.021746861210E+00
H	7.281107735120E-02	-1.836398819018E+00	-2.473531694490E+00
C	-3.527205751492E-01	2.268216649829E+00	2.549326086305E+00
H	2.042235896829E-01	-1.049010407695E+00	-1.511414692769E+00
H	-4.272611062447E-01	1.146736812697E+00	1.183752029090E+00
C	-2.784172910837E-01	1.813037281185E+00	1.993801392363E+00
C	-2.143421981214E-01	1.417481577404E+00	1.510049005808E+00
C	-2.777279080391E-01	3.617084908498E+00	4.192952627314E+00
C	-1.425580952334E-01	9.891875680931E-01	9.854261941305E-01
C	-2.130209331097E-01	4.004143688870E+00	4.664109738030E+00
C	-1.415309138239E-01	4.434781543027E+00	5.187699777846E+00
C	-7.679080868375E-02	4.824292534129E+00	5.655197604648E+00
C	-7.745476900699E-02	6.127489522145E-01	5.241918708926E-01
C	-7.610170433983E-02	6.631487339595E+00	7.852743169744E+00
C	-1.401968461030E-01	7.026040618435E+00	8.336607287461E+00
C	-2.119747203284E-01	7.454800346375E+00	8.860824491435E+00
C	-2.771053590861E-01	7.831680546101E+00	9.320670962380E+00
H	-2.958185338300E-01	9.501150777138E+00	1.135300125859E+01

Z2.5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
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16.35124189	500.00000000	500.00000000	90.000000	90.000000	90.000000
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ATOMS IN THE ASYMMETRIC UNIT 82 - ATOMS IN THE UNIT CELL: 82

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	-1.406594096661E-01	-2.653532421269E+00	-6.250926789379E-01
C	-2.121953984745E-01	-3.311928746303E+00	-7.807424447385E-01
C	-7.584767218769E-02	-2.062858151468E+00	-4.863296674642E-01
C	-2.768060835083E-01	-3.908138296604E+00	-9.190092009416E-01
C	-3.512398696540E-01	-4.590903459121E+00	-1.088555330613E+00
C	-4.263007241750E-01	-2.532815305427E+00	-6.001455921397E-01
C	-2.768098627780E-01	-6.656270994625E+00	-1.572878988941E+00
C	-3.512451934828E-01	-5.973620964269E+00	-1.402586381811E+00
C	-4.263056750444E-01	-3.903315033119E+00	-9.141906668148E-01
C	-4.263125531531E-01	-1.344812205366E+00	-3.195594412641E-01
C	-2.121863441670E-01	-7.251915538625E+00	-1.712125008975E+00
C	-1.406457007711E-01	-7.909466759936E+00	-1.869240138001E+00
C	-4.263130098365E-01	-2.824765867512E-02	-1.238160610377E-02
C	-4.263145714331E-01	-6.661098381007E+00	-1.576714593533E+00
C	4.986244097699E-01	-4.590843792880E+00	-1.088118422092E+00
C	-7.586976048431E-02	-8.500927921275E+00	-2.009071217289E+00
C	-4.263225329916E-01	1.160158324134E+00	2.664964919457E-01
C	4.986196766463E-01	-5.973585882889E+00	-1.402111196152E+00
C	-4.263313954746E-01	-8.031375192833E+00	-1.891691800323E+00

C 4.241810046098E-01 -3.908339153723E+00 -9.182724871282E-01
C -4.263136218740E-01 2.530169975866E+00 5.899554967406E-01
C -8.701480561372E-04 -1.057008302036E+01 -2.496848660278E+00
C -4.263421436336E-01 -9.218905803400E+00 -2.174297330132E+00
C 3.595482289439E-01 -3.312880197022E+00 -7.795351990801E-01
C 7.368208508876E-02 -1.123439046639E+01 -2.653114716697E+00
C -1.465901019209E-03 -9.185989333033E+00 -2.169709329414E+00
C 4.987983506599E-01 3.230417053505E+00 7.556760232116E-01
C -4.262863254393E-01 -1.582303963899E+01 -3.755526986718E+00
C -3.514116743572E-01 3.230207123115E+00 7.552229372673E-01
C -4.999791079956E-01 -1.515284448962E+01 -3.593555418250E+00
C 4.241819852296E-01 -6.656192499475E+00 -1.571779907264E+00
C -8.700699073068E-04 6.954807067446E-03 -9.902402040718E-04
C -3.526226451852E-01 -1.515186324905E+01 -3.594007708028E+00
C -1.445241056181E-03 -1.377565705008E+00 -3.262663844035E-01
C 7.367045738489E-02 6.717009385134E-01 1.550617816041E-01
C 4.987751659691E-01 -1.379073374079E+01 -3.265165955111E+00
C -4.263638363111E-01 -1.053473976309E+01 -2.484672069041E+00
C 2.880132804581E-01 -2.654695539464E+00 -6.233561335447E-01
C 1.482399582719E-01 -1.057033826292E+01 -2.496153605613E+00
C 7.372141688062E-02 -2.064755457365E+00 -4.870560665376E-01
C -3.514342906776E-01 -1.378968739192E+01 -3.265858839968E+00
C 7.368857700769E-02 -8.498901576223E+00 -2.006886903702E+00
C -4.263444290855E-01 -1.309081388493E+01 -3.096896703111E+00
C -4.263766340935E-01 -1.172213255388E+01 -2.767860484236E+00
C 1.482394831203E-01 7.647384394468E-03 -2.105164192085E-04
C 1.488625211689E-01 -1.376825236932E+00 -3.254195450674E-01
C 2.232720271820E-01 -2.062000468553E+00 -4.846810549123E-01
C 1.488416381353E-01 -9.186295736301E+00 -2.169101585819E+00
C -4.999721741602E-01 4.594020007139E+00 1.077779804342E+00
C 3.595496326253E-01 -7.251499114871E+00 -1.710955952205E+00
C -3.526160045473E-01 4.593815740928E+00 1.077356973168E+00
C 2.232426091823E-01 -8.501345414603E+00 -2.007967660270E+00
C 2.880005751848E-01 -7.909391844316E+00 -1.868225788560E+00
C -4.262886117988E-01 5.265405552824E+00 1.235943057249E+00
H 7.368034821249E-02 -1.228974621766E+01 -2.902714704194E+00
H -4.262631973262E-01 -1.687877802073E+01 -4.010499169258E+00
H 4.422489972163E-01 -1.567260744146E+01 -3.718802369062E+00
H -2.948280400250E-01 -1.567090853976E+01 -3.719396396489E+00
H 7.364480490834E-02 1.727482546062E+00 4.028644777405E-01
H 4.422490745014E-01 5.114021134651E+00 1.201162945840E+00
H -2.948280968049E-01 5.113626770497E+00 1.200404676651E+00
H -4.262805688018E-01 6.322379401394E+00 1.485754402263E+00
C -2.761867551230E-01 -1.311331973597E+01 -3.103710825839E+00
C -2.111398536111E-01 -1.253251890246E+01 -2.965071231436E+00
C -1.393842407872E-01 -1.187304306265E+01 -2.808060317814E+00
C -7.518399375112E-02 -1.126863099997E+01 -2.663004690368E+00
C -7.519092594172E-02 7.057894921615E-01 1.627155668057E-01
C -1.393345852538E-01 1.312511039959E+00 3.049348138431E-01

C	-2.111063369414E-01	1.972167359862E+00	4.595896053363E-01
C	-2.761571549181E-01	2.553383186796E+00	5.959354889660E-01
C	4.235029438338E-01	-1.311520961970E+01	-3.102721535192E+00
C	3.584638679625E-01	-1.253429763600E+01	-2.963524602269E+00
C	2.866950211242E-01	-1.187520913574E+01	-2.806128402679E+00
C	2.225495176922E-01	-1.126908532247E+01	-2.661676712052E+00
C	2.225378804990E-01	7.070826594902E-01	1.639747602834E-01
C	2.866893961115E-01	1.313556013319E+00	3.061509508278E-01
C	3.584632777214E-01	1.973054288134E+00	4.607251458438E-01
C	4.235292138197E-01	2.553904897287E+00	5.968326352058E-01
C	7.370305320820E-02	-7.127922659006E+00	-1.682303349199E+00
C	7.369290042685E-02	-5.940554210291E+00	-1.400922352534E+00
C	7.370215355265E-02	-4.623804636315E+00	-1.089915066270E+00
C	7.377983145508E-02	-3.435943308976E+00	-8.106687026300E-01

Z3

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35137871	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 100 - ATOMS IN THE UNIT CELL: 100

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
C	-7.707384229787E-02	3.732038435583E+00	9.666559276206E+00
C	-1.417123159904E-01	3.962874113423E+00	1.023263152980E+01
C	-2.132710080900E-01	4.216745395777E+00	1.085896163793E+01
C	-3.524537395790E-01	5.238179124834E+00	1.339182357162E+01
C	-2.779304577191E-01	4.445142612869E+00	1.142534915762E+01
C	-7.697059868189E-02	2.674374901245E+00	7.047396575729E+00
C	-4.275541722775E-01	5.514955642870E+00	1.404397147949E+01
C	-3.524018067016E-01	4.717693620079E+00	1.207271672413E+01
C	-1.417478555454E-01	2.441685209046E+00	6.486394238571E+00
C	4.973932866803E-01	5.238321149640E+00	1.339021473230E+01
C	-4.274565547356E-01	4.441038740908E+00	1.141905753628E+01
C	4.974405489256E-01	4.717659168100E+00	1.207126895740E+01
C	-4.274177944738E-01	3.920994887094E+00	1.011260166940E+01
C	-2.132884611315E-01	2.187229547080E+00	5.859574352034E+00
C	-4.274943930727E-01	3.460387267654E+00	8.982172688165E+00
C	-2.779751691441E-01	1.956782739721E+00	5.294393186441E+00
C	-4.275279371359E-01	2.952529800348E+00	7.728936835765E+00
C	-7.768562092173E-02	1.561436527906E-01	9.071582591238E-01
C	-4.275729028573E-01	2.491873400606E+00	6.598758827602E+00
C	-1.427316936495E-01	3.827339662032E-01	1.459568466642E+00
C	-3.523568733231E-01	1.689468231973E+00	4.642923478523E+00
C	-2.144905554891E-01	6.399050061704E-01	2.086608372805E+00
C	-4.275414907611E-01	1.958087930633E+00	5.295436082360E+00
C	-2.786238696040E-01	8.765661796840E-01	2.663323708354E+00
C	-3.529352914853E-01	1.149460693445E+00	3.327340266243E+00
C	4.973060896461E-01	1.690068362101E+00	4.641677801563E+00

C -4.274796604044E-01 8.906328455263E-01 2.695579643863E+00
C 4.979449350550E-01 1.150055154956E+00 3.326104057619E+00
H -4.274529253456E-01 4.790827509522E-01 1.692259983732E+00
C 4.236590037743E-01 8.772866354889E-01 2.661259560450E+00
C 3.594835345771E-01 6.405838238176E-01 2.085801602376E+00
C 7.247711613063E-02 1.162224449705E+00 3.362611988347E+00
C 7.243514615978E-02 6.986971477187E-01 2.233311946032E+00
C 7.249140081503E-02 1.676832871475E+00 4.612706955895E+00
C 4.228997536783E-01 1.957522047571E+00 5.292336213108E+00
C 2.877116098360E-01 3.834781419108E-01 1.459252809395E+00
C 3.581977069262E-01 2.188451183427E+00 5.856761373883E+00
C 7.255403395449E-02 2.137882550561E+00 5.743016580010E+00
C 2.866646827894E-01 2.442994713702E+00 6.483933686850E+00
C 7.252278181998E-02 2.676317309706E+00 7.041819109220E+00
C 2.220274969852E-01 2.675250868678E+00 7.049428685218E+00
C 2.226141674434E-01 1.569959162683E-01 9.083961293654E-01
C -2.568366680823E-03 2.931993727454E+00 7.702825044063E+00
C 1.475804599890E-01 2.932519825338E+00 7.703574129009E+00
C 7.246069700048E-02 1.653335621441E-01 9.305152993105E-01
C -2.604747915140E-03 3.476706910717E+00 9.012104135948E+00
C 1.473665570355E-01 -1.068237876628E-01 2.649400574204E-01
C 1.475491276543E-01 3.477022126375E+00 9.012944951901E+00
C 7.245858482639E-02 3.733306354432E+00 9.673626024466E+00
C -2.416493277696E-03 -1.072749361381E-01 2.642748923303E-01
C 2.219970168392E-01 3.733016460417E+00 9.667824963038E+00
C 2.867154430615E-01 3.962830421502E+00 1.023185280726E+01
C 3.583080271117E-01 4.216626881599E+00 1.085741255201E+01
C 1.461810025607E-01 -6.367834893650E-01 -1.032101422108E+00
C -1.175362761952E-03 -6.376239078445E-01 -1.032593999632E+00
C 4.230088677843E-01 4.445126374605E+00 1.142256021368E+01
C 7.251685819004E-02 -8.983092000859E-01 -1.670942692502E+00
H 2.039824882339E-01 -8.377340346000E-01 -1.526627183724E+00
H -5.895155907594E-02 -8.393543434319E-01 -1.527489304933E+00
H 7.254113581083E-02 -1.308246175530E+00 -2.676588325438E+00
C -2.626705313269E-03 6.481120378973E+00 1.644996477951E+01
C -2.128464100604E-03 7.008454899939E+00 1.777070972937E+01
C 7.243378770475E-02 4.270343150162E+00 1.097315465682E+01
C 7.250174501969E-02 4.727859066328E+00 1.210488678663E+01
C 7.256046628084E-02 5.236747616337E+00 1.335750754185E+01
C 7.267378999649E-02 5.693929866082E+00 1.448911219222E+01
C 7.259098921793E-02 6.219219847394E+00 1.579590165467E+01
C -7.647641809714E-02 7.273852615983E+00 1.843664763949E+01
C 7.238245694014E-02 7.260883014279E+00 1.840616172285E+01
C 1.477031154897E-01 6.480971111687E+00 1.645317215746E+01
C 1.469897427570E-01 7.008369948947E+00 1.777387785931E+01
C -1.406021046819E-01 7.503758013682E+00 1.901628981429E+01
C -7.695534487997E-02 6.219844655035E+00 1.579453826728E+01
C 2.221493916402E-01 6.220071398493E+00 1.580116832931E+01
C 2.212520079527E-01 7.274166333268E+00 1.844219183989E+01

C	-2.123722914539E-01	7.754040724365E+00	1.964607006883E+01
C	2.854413011228E-01	7.504514699046E+00	1.901975793589E+01
C	-2.774163336545E-01	7.974088666996E+00	2.020115634837E+01
C	2.868233286080E-01	5.992412238497E+00	1.523449613210E+01
C	-3.538230874344E-01	8.752005118892E+00	2.214840596701E+01
C	-1.418351924713E-01	5.990904420878E+00	1.523466129869E+01
C	-3.526525907165E-01	8.231554321487E+00	2.084748068956E+01
C	-4.274756980984E-01	9.007480723601E+00	2.278997642718E+01
C	3.572227545459E-01	7.754763977422E+00	1.964916011076E+01
C	4.988244218048E-01	8.751219467286E+00	2.215010502382E+01
C	-4.275672853510E-01	7.964514640080E+00	2.018014057720E+01
C	4.222915217866E-01	7.974987032709E+00	2.020342988549E+01
C	4.975656614519E-01	8.231686163454E+00	2.084886025153E+01
C	3.583371379150E-01	5.737803249526E+00	1.460688493379E+01
C	-4.276194270422E-01	7.441968818660E+00	1.887300243381E+01
C	-4.276229018645E-01	6.989168135165E+00	1.773937641292E+01
C	4.229467490024E-01	5.510175987966E+00	1.403863491256E+01
C	-2.133777337590E-01	5.736393225192E+00	1.460831771419E+01
C	-4.276103936807E-01	6.488402256451E+00	1.648366116872E+01
C	-4.276061605062E-01	6.032580719954E+00	1.535122183847E+01
C	-2.780571908326E-01	5.509223330827E+00	1.404209410016E+01
H	7.229864230049E-02	7.662035938095E+00	1.941360309024E+01
H	-2.960202011924E-01	8.951329207628E+00	2.264348192503E+01
H	-4.274389715285E-01	9.410467445407E+00	2.379852716907E+01
H	4.410554439560E-01	8.948956612558E+00	2.264687673406E+01

Z3.5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35111230	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 118 - ATOMS IN THE UNIT CELL: 118					
ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)		

C	2.858718824578E-01	-2.880638654097E+00	-1.505331897179E-01		
C	3.574120496751E-01	-3.555929383213E+00	-1.860931557746E-01		
C	2.211259999488E-01	-2.272879601762E+00	-1.167915874239E-01		
C	4.220716691177E-01	-4.165639227693E+00	-2.213734200000E-01		
C	4.964974150077E-01	-4.868554101925E+00	-2.511427224690E-01		
C	1.467301487117E-01	-1.570224254565E+00	-7.754067289898E-02		
C	-4.283987959287E-01	-2.756725845481E+00	-1.396846632426E-01		
C	4.220150353293E-01	-6.985683753861E+00	-3.702719229515E-01		
C	4.964763188263E-01	-6.283728486558E+00	-3.396104191204E-01		
C	-4.284156035946E-01	-4.160035631205E+00	-2.241842978202E-01		
C	-4.284103709406E-01	-1.537721106583E+00	-7.380075104261E-02		
C	3.574057430556E-01	-7.596923231221E+00	-4.058200188895E-01		
C	2.858334132993E-01	-8.271749284542E+00	-4.403803371392E-01		
C	-4.284182177251E-01	-1.879145786701E-01	1.300889696312E-03		

C 1.461293990880E-01 -1.501765747763E-01 -6.015591693228E-04
C -4.284445635841E-01 -6.992631679309E+00 -3.662107986599E-01
C -3.533439719334E-01 -4.869041602034E+00 -2.512075928535E-01
C 7.156200082508E-02 -2.275227785261E+00 -1.152906369842E-01
C 2.211472300627E-01 -8.880818885178E+00 -4.758462961630E-01
C -4.284409640421E-01 1.031094548824E+00 6.587816368829E-02
C -3.533493529880E-01 -6.284224765468E+00 -3.396877559989E-01
C -4.284645522038E-01 -8.395755111194E+00 -4.497182254660E-01
C -2.789071247878E-01 -4.166473009678E+00 -2.213554507057E-01
C 1.466707440880E-01 -9.582382633857E+00 -5.073152361280E-01
C -4.284374715952E-01 2.436899821655E+00 1.391002426458E-01
C -4.283928166460E-01 -9.615030323533E+00 -5.139732859689E-01
C -2.142715647252E-01 -3.556094784844E+00 -1.863042595288E-01
C 1.466367045555E-01 -1.099785081192E+01 -5.953828368843E-01
C 7.160743305540E-02 -8.873264395696E+00 -4.789989628722E-01
C -3.535430560549E-01 3.155350834242E+00 1.761642063154E-01
C 4.966711904346E-01 3.155438112610E+00 1.763220456403E-01
C -2.789034547769E-01 -6.986627043387E+00 -3.702106666748E-01
C -4.283708966812E-01 -1.096411719025E+01 -5.893265034378E-01
C -1.427398501950E-01 -2.880467616501E+00 -1.507369889430E-01
C -4.283671899626E-01 -1.218341009233E+01 -6.525880643742E-01
C -7.800276818052E-02 -2.272494871517E+00 -1.170147294905E-01
C 7.153711212689E-02 -1.170592679453E+01 -6.235038517436E-01
C -3.493678591738E-03 -9.581357236929E+00 -5.074102933083E-01
C -3.547538384520E-01 4.554617539513E+00 2.487176733783E-01
C -2.142645556473E-01 -7.597008417053E+00 -4.061920435314E-01
C 4.978891806871E-01 4.554701679425E+00 2.488043163623E-01
C -7.794130270460E-02 -8.878947671014E+00 -4.761467675903E-01
C -3.526992628153E-03 -1.099681678787E+01 -5.955246574636E-01
C -1.426790248935E-01 -8.271329074029E+00 -4.406602518632E-01
C -4.284305407492E-01 5.243645480215E+00 2.846912451375E-01
C 7.157131540090E-02 5.311801608879E-01 3.668418168834E-02
C -3.601559635311E-03 -1.570023738521E+00 -7.759446006836E-02
C -2.992531301280E-03 -1.499819767228E-01 -6.468501523611E-04
H -2.969639905665E-01 5.088039287505E+00 2.761910955757E-01
H 4.401023190649E-01 5.088210630182E+00 2.762423215998E-01
H -4.284277979668E-01 6.328256260944E+00 3.412253753372E-01
H 7.157751275949E-02 1.614034198162E+00 9.585814087794E-02
C 7.164552227743E-02 -7.469615105685E+00 -3.950546774289E-01
C 7.160487524130E-02 -6.250563002369E+00 -3.301317085871E-01
C 7.158204677359E-02 -4.900473469876E+00 -2.555153973275E-01
C 7.155250511072E-02 -3.681717468909E+00 -1.899693200566E-01
C 2.204316590469E-01 5.669497809188E-01 3.820818169688E-02
C 2.845925449928E-01 1.188712528459E+00 7.173072168947E-02
C 3.563585177586E-01 1.865245655177E+00 1.079170833288E-01
C 4.214092584265E-01 2.461383950951E+00 1.396616919521E-01
C -7.729583145941E-02 5.671035165177E-01 3.818066101761E-02
C -1.414423262734E-01 1.189249420136E+00 7.168218104706E-02
C -2.132162862068E-01 1.865601495749E+00 1.077947113482E-01

C -2.782848135863E-01 2.461219311676E+00 1.395025745484E-01
C 4.964818995729E-01 -1.571030499607E+01 -8.458405481071E-01
C -4.283995051829E-01 -1.358666731636E+01 -7.343013978162E-01
C -3.533602538107E-01 -1.571110826669E+01 -8.456791846575E-01
C -4.284794055317E-01 -1.782302001849E+01 -9.529618125835E-01
C 4.220587655885E-01 -1.359236819055E+01 -7.305342299616E-01
C -2.788560557003E-01 -1.359393892713E+01 -7.302414505180E-01
C -4.284393495441E-01 -2.039214108164E+01 -1.086873110380E+00
C 2.858057045523E-01 -1.230837278876E+01 -6.615725447437E-01
C 2.210814275073E-01 -1.170035677688E+01 -6.264753641225E-01
C -1.427123497142E-01 -1.230689557640E+01 -6.618188062642E-01
C -4.284353998873E-01 -2.161129392401E+01 -1.148607029693E+00
C -7.800309866282E-02 -1.169840305438E+01 -6.267473373089E-01
C -4.284437416990E-01 -1.904214429452E+01 -1.015421913365E+00
C -4.284301281681E-01 -2.301728053728E+01 -1.218237639042E+00
C -4.284236634936E-01 -2.582440990769E+01 -1.356355885333E+00
C 4.966788938868E-01 -2.373592623862E+01 -1.253530389269E+00
C -3.535354646058E-01 -2.373582332101E+01 -1.253454780148E+00
C 4.978962503042E-01 -2.513538062092E+01 -1.322318960407E+00
C -3.547470655250E-01 -2.513527442411E+01 -1.322349051527E+00
C 3.573948209090E-01 -1.298267169979E+01 -6.954229027740E-01
C 7.150083202009E-02 -1.310964758897E+01 -7.062185590572E-01
C -2.142793114512E-01 -1.298176214791E+01 -6.956438535939E-01
C -2.782762866903E-01 -2.304162286021E+01 -1.218515961429E+00
C 4.214178532176E-01 -2.304179543074E+01 -1.218652436737E+00
C 7.157108932250E-02 -1.432880446912E+01 -7.689641347769E-01
C 3.563547401964E-01 -2.244594337169E+01 -1.188587952541E+00
C -2.132255334924E-01 -2.244540275905E+01 -1.188384787381E+00
C 7.158651991409E-02 -1.567907972668E+01 -8.410713108937E-01
C 2.845836112462E-01 -2.176943004517E+01 -1.154184840912E+00
C 3.573959741447E-01 -1.702297595934E+01 -9.079015346095E-01
C -1.414564959518E-01 -2.176885974164E+01 -1.154011590304E+00
C -2.142747508725E-01 -1.702389523192E+01 -9.078115047134E-01
C 7.159611534242E-02 -1.689795797663E+01 -9.039282211675E-01
C 2.204319196841E-01 -2.114733036455E+01 -1.122167671535E+00
C -7.729743445366E-02 -2.114699088715E+01 -1.122167719779E+00
C 1.467427315384E-01 -1.900990149528E+01 -1.011707101932E+00
C 2.211414092042E-01 -1.830729099438E+01 -9.740550385471E-01
C 2.858668997072E-01 -1.769886726296E+01 -9.418059835288E-01
C 7.158226634858E-02 -1.830459356840E+01 -9.756208119971E-01
C 1.461309810780E-01 -2.043010782664E+01 -1.085140311632E+00
C 7.156666084855E-02 -2.111135815019E+01 -1.120729442513E+00
C -3.588239618094E-03 -1.900964597480E+01 -1.011744714091E+00
C -1.427335255525E-01 -1.769921258396E+01 -9.417526110384E-01
C -2.991076557121E-03 -2.042988996906E+01 -1.085158186427E+00
C -7.798354772885E-02 -1.830690634448E+01 -9.740876752880E-01
C 4.220404501259E-01 -1.641276862114E+01 -8.742907172269E-01
C -2.789426159137E-01 -1.641433268260E+01 -8.740026837328E-01
C 4.964998117231E-01 -1.429496137210E+01 -7.598798426211E-01

C -4.284525375756E-01 -1.641950632558E+01 -8.715125550876E-01
 C -3.533254028209E-01 -1.429576209788E+01 -7.597503236823E-01
 H -4.284208851778E-01 -2.690916048401E+01 -1.410007007371E+00
 H 4.401089711260E-01 -2.566894276466E+01 -1.348464679748E+00
 H -2.969572404646E-01 -2.566875701823E+01 -1.348635212266E+00
 H 7.156067673996E-02 -2.219437109370E+01 -1.176909100476E+00

Z4

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083

ANGSTROM

PRIMITIVE CELL

A	B	C	ALPHA	BETA	GAMMA
16.35115399	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 136 - ATOMS IN THE UNIT CELL: 136

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
C	-6.919558506351E-02	5.861620103489E+00	8.948618379242E+00
C	-1.338924144952E-01	6.192314027576E+00	9.460840450717E+00
C	-2.054728124441E-01	6.554777756193E+00	1.003098293856E+01
C	-3.445252809338E-01	8.033950848225E+00	1.232867314097E+01
C	-2.701227159783E-01	6.886581634329E+00	1.054397803430E+01
C	-6.906729141135E-02	4.341238363593E+00	6.568796317600E+00
C	-4.196087339978E-01	8.407612301151E+00	1.293203898721E+01
C	-3.445582780126E-01	7.260811531602E+00	1.114000917722E+01
C	-1.338242900967E-01	4.008711077742E+00	6.059829256773E+00
C	-4.947232136020E-01	8.036042254777E+00	1.232860220357E+01
C	-4.196680506185E-01	6.889608919272E+00	1.053633986671E+01
C	-4.947413939408E-01	7.262013478639E+00	1.114048503042E+01
C	-4.197040125855E-01	6.124822480783E+00	9.356498573501E+00
C	-2.053594130041E-01	3.644590357462E+00	5.489789899567E+00
C	-4.196402183006E-01	5.467189252916E+00	8.327905218403E+00
C	-2.700779630569E-01	3.315216097040E+00	4.976965199998E+00
C	-4.196402514407E-01	4.735517079924E+00	7.190850241622E+00
C	-6.976787014262E-02	7.595136698847E-01	9.821140729792E-01
C	-4.196397301164E-01	4.076563888789E+00	6.163565518287E+00
C	-1.348238614804E-01	1.080674129782E+00	1.485183968789E+00
C	-3.444494987139E-01	2.935157416213E+00	4.383954340081E+00
C	-2.065853063836E-01	1.445249583173E+00	2.056345858153E+00
C	-4.196305407036E-01	3.316901948428E+00	4.977529531272E+00
C	-2.707138182227E-01	1.781296298849E+00	2.581638506328E+00
C	-3.450264227975E-01	2.168340866511E+00	3.186284295709E+00
C	-4.947856461470E-01	2.936114622697E+00	4.382635288581E+00
C	-4.195801847506E-01	1.800394797594E+00	2.611422624092E+00
C	-4.941543384947E-01	2.169027194425E+00	3.185098032719E+00
H	-4.195607524190E-01	1.215865777439E+00	1.697950437420E+00
C	4.315547140556E-01	1.782365767928E+00	2.579576532266E+00
C	3.674018967509E-01	1.447017289739E+00	2.054774979898E+00

C 8.037988362678E-02 2.187459898798E+00 3.218226970902E+00
C 8.039098783516E-02 1.529626793239E+00 2.189831611824E+00
C 8.039440956757E-02 2.918033475115E+00 4.355881267740E+00
C 4.308077746391E-01 3.316971937145E+00 4.974011828722E+00
C 2.956213528307E-01 1.082250657024E+00 1.484165766975E+00
C 3.661039799956E-01 3.646756711797E+00 5.487168017035E+00
C 8.043610692917E-02 3.575419596855E+00 5.384531216713E+00
C 2.945858543995E-01 4.010940464137E+00 6.057418897879E+00
C 8.041208944496E-02 4.341494367355E+00 6.563214920187E+00
C 2.299023644168E-01 4.341767846509E+00 6.570035686039E+00
C 2.305486021985E-01 7.607825896279E-01 9.819586307004E-01
C 5.319039215632E-03 4.714013649550E+00 7.166355310403E+00
C 1.554799253121E-01 4.714618950510E+00 7.166583028613E+00
C 8.039312525846E-02 7.728492819865E-01 1.002883813414E+00
C 5.282851770883E-03 5.489586115821E+00 8.353436363917E+00
C 1.552906326888E-01 3.865359404235E-01 3.961479227548E-01
C 1.554562546010E-01 5.491268236636E+00 8.352872901375E+00
C 8.035906963084E-02 5.863070122849E+00 8.956427986474E+00
C 5.501339419369E-03 3.862139167057E-01 3.960269270809E-01
C 2.298946973219E-01 5.865064058254E+00 8.948269504992E+00
C 2.945373260711E-01 6.197306575372E+00 9.461449714296E+00
C 3.661124839119E-01 6.559407208895E+00 1.003175008396E+01
C 1.540860975969E-01 -3.662224865030E-01 -7.856122338381E-01
C 6.727496709086E-03 -3.668396525780E-01 -7.855351719693E-01
C 4.307820114088E-01 6.889498545090E+00 1.054534736539E+01
C 8.041129005675E-02 -7.377936401032E-01 -1.367023297975E+00
H 2.118766209831E-01 -6.522458268254E-01 -1.236627835615E+00
H -5.105478477961E-02 -6.540114055501E-01 -1.236089934314E+00
H 8.041952141770E-02 -1.321803397336E+00 -2.282696679046E+00
C 5.246072090964E-03 9.805740830766E+00 1.511663661312E+01
C 5.256599069145E-03 1.055722149604E+01 1.631930216813E+01
C 8.037304041002E-02 6.628919751988E+00 1.013540755422E+01
C 8.050465345200E-02 7.285366772834E+00 1.116476382815E+01
C 8.048735055639E-02 8.012229086029E+00 1.230393932797E+01
C 8.033539354684E-02 8.669419545225E+00 1.333289608082E+01
C 8.032753398192E-02 9.415536668262E+00 1.452427083382E+01
C -6.918481377078E-02 1.094007978062E+01 1.690867237698E+01
C 8.035367232723E-02 1.094663235665E+01 1.691156536196E+01
C 1.554373494551E-01 9.806142447583E+00 1.511578352990E+01
C 1.554366944720E-01 1.055643413537E+01 1.631915531381E+01
C -1.338724872829E-01 1.126506429906E+01 1.742503480447E+01
C -6.922546881626E-02 9.420995777030E+00 1.452907621047E+01
C 2.298788213893E-01 9.423005535865E+00 1.452623745475E+01
C 2.298774695147E-01 1.094029524373E+01 1.690833753960E+01
C -2.054594507523E-01 1.162912545203E+01 1.799364254586E+01
C 2.946471502102E-01 1.126406141968E+01 1.742242746526E+01
C -2.700966050246E-01 1.195487971396E+01 1.851114988368E+01
C 2.945892751152E-01 9.097687586143E+00 1.401089160634E+01
C -3.445978051124E-01 1.308313729226E+01 2.030642577172E+01

C	-1.339944415742E-01	9.097170429375E+00	1.401474780415E+01
C	-3.445506044013E-01	1.233692143249E+01	1.910064691841E+01
C	-4.196910670597E-01	1.347050564772E+01	2.089998411870E+01
C	3.662328196606E-01	1.162822164515E+01	1.799104423738E+01
C	-4.947591286089E-01	1.308290782968E+01	2.030552900779E+01
C	-4.196238261740E-01	1.194907460783E+01	1.850650245089E+01
C	4.308404290771E-01	1.195485492033E+01	1.850891211113E+01
C	-4.947302686299E-01	1.233670507043E+01	1.909982956634E+01
C	3.661566914874E-01	8.735534435493E+00	1.344034082138E+01
C	-4.195832363337E-01	1.120610605791E+01	1.731315924862E+01
C	-4.196392377145E-01	1.055104421921E+01	1.628269991299E+01
C	4.308401732724E-01	8.406807073682E+00	1.292635600286E+01
C	-2.055256756978E-01	8.734563109352E+00	1.344380671007E+01
C	-4.196477386312E-01	9.826565378275E+00	1.514238105090E+01
C	-4.195641142758E-01	9.171860591265E+00	1.411177123833E+01
C	-2.700783444958E-01	8.404024127881E+00	1.292656075016E+01
C	5.759271467011E-03	1.561078163568E+01	2.429891322787E+01
C	5.149460442376E-03	1.485250668117E+01	2.309569009976E+01
C	8.032082914646E-02	1.597435563230E+01	2.487599771799E+01
C	8.031303849729E-02	1.447533864688E+01	2.249852528560E+01
C	1.548849416228E-01	1.561068906103E+01	2.429840400579E+01
C	8.030045694882E-02	1.372253301611E+01	2.130801265775E+01
C	8.023474805409E-02	1.306959420835E+01	2.027682527222E+01
C	1.554886486875E-01	1.485170311977E+01	2.309563155788E+01
C	2.291900926216E-01	1.599368738280E+01	2.490569428605E+01
C	8.022192115078E-02	1.234776507442E+01	1.913346970956E+01
C	8.038965904268E-02	1.169332788129E+01	1.810290595527E+01
C	2.933670843972E-01	1.632649415714E+01	2.543149364319E+01
C	2.298729218105E-01	1.447699552614E+01	2.249946456271E+01
C	-6.925583207432E-02	1.447808134476E+01	2.249970084689E+01
C	-6.853980487322E-02	1.599245384274E+01	2.490698503417E+01
C	3.651298480447E-01	1.668722646285E+01	2.600495580808E+01
H	8.033465079233E-02	1.655113490195E+01	2.579435446284E+01
C	-1.326852764473E-01	1.632454010078E+01	2.543418944876E+01
C	4.301895746559E-01	1.700499357232E+01	2.650989779751E+01
C	-1.339992807012E-01	1.415319086435E+01	2.198498250610E+01
C	-4.933816765941E-01	1.812156132493E+01	2.828464236671E+01
C	2.946551848434E-01	1.415342154568E+01	2.198518416853E+01
C	-4.945718081940E-01	1.737474108145E+01	2.709908359161E+01
C	-4.197139736554E-01	1.848929352019E+01	2.886875830186E+01
C	-2.044540219890E-01	1.668548000712E+01	2.600766179096E+01
C	-3.460210425207E-01	1.812124254214E+01	2.828558373940E+01
C	-4.196660036428E-01	1.699045600539E+01	2.649124140580E+01
C	-2.695165450773E-01	1.700334715250E+01	2.651263391523E+01
C	-3.447870430962E-01	1.737412692349E+01	2.710024627527E+01
C	-2.055162294004E-01	1.379098481867E+01	2.141332106330E+01
C	-4.196386303274E-01	1.623862766080E+01	2.530110947232E+01
C	-4.197101114900E-01	1.558684222868E+01	2.426877954222E+01
C	-2.702001871038E-01	1.346678107530E+01	2.089687625201E+01

C	3.661884845087E-01	1.379089417399E+01	2.141366140099E+01
C	-4.197204272680E-01	1.486674488498E+01	2.312479071658E+01
C	-4.197146422093E-01	1.421377188978E+01	2.209324153932E+01
C	4.307958745682E-01	1.346554000389E+01	2.089541763334E+01
H	4.488229033205E-01	1.840576915735E+01	2.873660504173E+01
H	-4.197363205774E-01	1.906858283856E+01	2.978748363806E+01
H	-2.882387380440E-01	1.840593493816E+01	2.873786855008E+01

Z4.5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35104315	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 154 - ATOMS IN THE UNIT CELL: 154

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
C	-1.421624232146E-01	2.960667712918E+00	4.239699973213E-01
C	-2.136940892729E-01	3.628915530090E+00	5.287882962947E-01
C	-7.743051364865E-02	2.359196626777E+00	3.279998800889E-01
C	-2.783579496728E-01	4.231601887575E+00	6.264992675019E-01
C	-3.527761562783E-01	4.927861749316E+00	7.286344862960E-01
C	-4.278889593665E-01	2.839018305655E+00	3.995500432602E-01
C	-2.782760178136E-01	7.021335045222E+00	1.064542694826E+00
C	-3.527414058283E-01	6.326117653082E+00	9.640020399343E-01
C	-4.278690596514E-01	4.225930537663E+00	6.293940375904E-01
C	-4.278584388903E-01	1.633461635064E+00	2.074309117726E-01
C	-2.136889530179E-01	7.626336583358E+00	1.161459979361E+00
C	-1.421128934009E-01	8.293652165500E+00	1.267287440267E+00
C	-4.278622562902E-01	2.988327306367E-01	-8.049694480676E-03
C	-4.278153563457E-01	7.028508746191E+00	1.064263519115E+00
C	4.970628051362E-01	4.928571885806E+00	7.290428159098E-01
C	-7.734403691787E-02	8.893956841473E+00	1.361949515773E+00
C	-4.278445061113E-01	-9.066946487685E-01	-1.999660156022E-01
C	4.970861304081E-01	6.326829784448E+00	9.644372225304E-01
C	-4.277899469665E-01	8.414963235407E+00	1.296038525210E+00
C	4.226263613389E-01	4.232874254078E+00	6.270951365692E-01
C	-4.278489625470E-01	-2.297263119436E+00	-4.192394698710E-01
C	-2.942050112634E-03	1.098919428476E+01	1.693735174692E+00
C	-4.277965103649E-01	9.620673935823E+00	1.488170745478E+00
C	3.580097859200E-01	3.628801570136E+00	5.293807027623E-01
C	7.213330261324E-02	1.168804108579E+01	1.816224881486E+00
C	-2.906494881448E-03	9.587019875667E+00	1.481568475635E+00
C	4.972578155119E-01	-3.007928679149E+00	-5.309619902088E-01
C	-3.529555276523E-01	-3.007932936810E+00	-5.313051181545E-01
C	4.226585277338E-01	7.023031845760E+00	1.065764871390E+00
C	-2.404312852690E-03	2.606753015167E-01	-9.772574072537E-03
C	-3.022946439876E-03	1.664692093815E+00	2.163296899726E-01
C	7.216595597729E-02	-4.126565290981E-01	-1.183988954651E-01

C -4.277753613180E-01 1.095496019175E+01 1.701304259415E+00
C 2.864687330693E-01 2.960462402396E+00 4.246767333663E-01
C 1.472457696968E-01 1.098999378447E+01 1.694315084278E+00
C 7.213595074564E-02 2.361953072523E+00 3.288482381001E-01
C 7.220201779760E-02 8.888887747401E+00 1.360134174296E+00
C -4.277080612710E-01 1.216059052467E+01 1.894127895772E+00
C 1.467198483449E-01 2.610920325108E-01 -9.478256490962E-03
C 1.473097470896E-01 1.665124542988E+00 2.166806947541E-01
C 2.217085905806E-01 2.359773471666E+00 3.288817727604E-01
C 1.472725966577E-01 9.587884577468E+00 1.482257684112E+00
C 4.984696055930E-01 -4.391963932597E+00 -7.491986211819E-01
C 3.580449156104E-01 7.627286790583E+00 1.163143365972E+00
C -3.541698060953E-01 -4.391972766517E+00 -7.494901636435E-01
C 2.217489533951E-01 8.895795572061E+00 1.363432825047E+00
C 2.864798845181E-01 8.294386051312E+00 1.269061565194E+00
C -4.278511831665E-01 -5.073471959825E+00 -8.565371332518E-01
H 7.217948378124E-02 -1.483316209439E+00 -2.908664945051E-01
H 4.406872716919E-01 -4.919789572272E+00 -8.322976955391E-01
H -2.963890512441E-01 -4.919812548332E+00 -8.327953589512E-01
H -4.278529441151E-01 -6.146380386076E+00 -1.025110448602E+00
C -7.669986187158E-02 -4.485251487246E-01 -1.238508085360E-01
C -1.408900007637E-01 -1.062467177646E+00 -2.225749814133E-01
C -2.126540254746E-01 -1.731543472985E+00 -3.292208377709E-01
C -2.776981849880E-01 -2.321326171151E+00 -4.227639920956E-01
C 2.210279491096E-01 -4.477920282491E-01 -1.232599108046E-01
C 2.851691945827E-01 -1.063182531653E+00 -2.215290286753E-01
C 3.569395535846E-01 -1.732187403608E+00 -3.281619589605E-01
C 4.220009476405E-01 -2.321395657784E+00 -4.220256152272E-01
C 7.224324867270E-02 7.499048380194E+00 1.147183932894E+00
C 7.205265515345E-02 6.293537970667E+00 9.548538219407E-01
C 7.204597008117E-02 4.957919153045E+00 7.439441346739E-01
C 7.210524775401E-02 3.752609425469E+00 5.520507362874E-01
C -3.527695900112E-01 1.565158729692E+01 2.440300934728E+00
C -4.277711715852E-01 1.355005624520E+01 2.106106091214E+00
C 4.970342474806E-01 1.564964648852E+01 2.440382267994E+00
C -4.279713148554E-01 1.773854507580E+01 2.774991413596E+00
C -2.782305528935E-01 1.355734906032E+01 2.110966580535E+00
C 4.226831936635E-01 1.355368420613E+01 2.110896701274E+00
C -4.277798595447E-01 2.027783443790E+01 3.184328225552E+00
C -1.421236520562E-01 1.228365433834E+01 1.906147717950E+00
C -7.741477401212E-02 1.168153151544E+01 1.811642864375E+00
C 2.864121587556E-01 1.228481859056E+01 1.907192059029E+00
C -4.279585830356E-01 2.148307898596E+01 3.379508745468E+00
C 2.216816621653E-01 1.168329979444E+01 1.812691859531E+00
C -4.277883724332E-01 1.894404342139E+01 2.968736371297E+00
C -4.278983561130E-01 2.286885487900E+01 3.615262676475E+00
C -4.277793448817E-01 2.566954322210E+01 4.062694967522E+00
C -3.527842907449E-01 2.356954373044E+01 3.718364327391E+00
C 4.970492571166E-01 2.357126510288E+01 3.719150093506E+00

C -3.527294111122E-01 2.496690672515E+01 3.959172557949E+00
C 4.971141975447E-01 2.496861720302E+01 3.959972698158E+00
C -2.136842871981E-01 1.295075169390E+01 2.015628298200E+00
C 3.579893865229E-01 1.295118690571E+01 2.016488272715E+00
C 4.225657149593E-01 2.287738717445E+01 3.614145846064E+00
C -2.783591412100E-01 2.287381957239E+01 3.612911766881E+00
C 7.210431854369E-02 1.307757544868E+01 2.029231573795E+00
C -2.137139813067E-01 2.227094855859E+01 3.512299958577E+00
C 3.579712170965E-01 2.227312768502E+01 3.513535543151E+00
C 7.224390838603E-02 1.428307919774E+01 2.223215582850E+00
C -1.421236594813E-01 2.160441062697E+01 3.406620318844E+00
C -2.137275247680E-01 1.694950245953E+01 2.655858862204E+00
C 2.864082698373E-01 2.160549920781E+01 3.407697719326E+00
C 3.579201715570E-01 1.694500765918E+01 2.656572228132E+00
C -7.736155387635E-02 2.100461111768E+01 3.307376254413E+00
C 7.225494509244E-02 1.561736771455E+01 2.437320724533E+00
C 2.217224459436E-01 2.100366350445E+01 3.308040085039E+00
C -7.739363023254E-02 1.821619038291E+01 2.861838963526E+00
C -1.421582452100E-01 1.761635571099E+01 2.763176530277E+00
C 7.216549670859E-02 1.682310451068E+01 2.629824193576E+00
C 1.472681853692E-01 2.030889278299E+01 3.202561737426E+00
C 7.218515409057E-02 2.101082475707E+01 3.304683833212E+00
C 7.215752666475E-02 1.820947009226E+01 2.862567242891E+00
C 2.863641148351E-01 1.761254057609E+01 2.764079213872E+00
C 1.472614655319E-01 1.891087942363E+01 2.965382155576E+00
C -2.929855216993E-03 1.891126774607E+01 2.964904524783E+00
C -2.912311187487E-03 2.030941067547E+01 3.202219902902E+00
C 2.216980770989E-01 1.821524377454E+01 2.862330747609E+00
C -2.783554223758E-01 1.634522841980E+01 2.560371588976E+00
C 4.225504766235E-01 1.634101115190E+01 2.560485398984E+00
C -3.527032515001E-01 1.424938646596E+01 2.229578432659E+00
C -4.279034085857E-01 1.634900645420E+01 2.563313282069E+00
C 4.971016588839E-01 1.424736012897E+01 2.229696868823E+00
C -4.278231119343E-01 3.496564656955E+01 5.569115825511E+00
C 4.984852989869E-01 3.428464349201E+01 5.460904958776E+00
C -3.541554364017E-01 3.428397494123E+01 5.460788933146E+00
C 4.972470291290E-01 3.290091234589E+01 5.240854745489E+00
C -3.529658951501E-01 3.290026299820E+01 5.240481280245E+00
C 4.219762937162E-01 3.221492059719E+01 5.131046152137E+00
C -2.777130011839E-01 3.221379897858E+01 5.130229693929E+00
C 3.569692117670E-01 3.162423437397E+01 5.036433022175E+00
C -4.278723389879E-01 3.219012093751E+01 5.127468530210E+00
C -2.126286400632E-01 3.162541106294E+01 5.035378887958E+00
C 7.221946405735E-02 2.239758582242E+01 3.536911870156E+00
C 7.219260898335E-02 3.030606419362E+01 4.823077465373E+00
C 2.852131303071E-01 3.095509255438E+01 4.928491517847E+00
C -1.408435129365E-01 3.095709054343E+01 4.927691905539E+00
C 2.210572954180E-01 3.034037845711E+01 4.828622648432E+00
C -2.389279800913E-03 2.963326513562E+01 4.713368190919E+00

C	-7.667602317909E-02	3.034252612025E+01	4.828706600657E+00
C	1.467373049885E-01	2.963207900639E+01	4.713314593565E+00
C	-4.278989737175E-01	3.079994249547E+01	4.905811414430E+00
C	7.213192093474E-02	2.360261778274E+01	3.732097439516E+00
C	-3.035937805046E-03	2.822952007853E+01	4.485406822481E+00
C	1.472991931422E-01	2.822835086014E+01	4.485392142749E+00
C	7.211021122516E-02	2.753204341859E+01	4.372044273288E+00
C	-4.278666023519E-01	2.959488321454E+01	4.710939647655E+00
C	7.212301521346E-02	2.493698240056E+01	3.951159491150E+00
C	7.207549972279E-02	2.614172068431E+01	4.146713567675E+00
C	2.216802682968E-01	2.753351621091E+01	4.370953204973E+00
C	-7.745692022920E-02	2.753590430736E+01	4.370693842956E+00
C	2.864619207851E-01	2.693377721602E+01	4.273217370429E+00
C	-1.421248235601E-01	2.693302222380E+01	4.272290938973E+00
C	-4.278479596401E-01	2.826069313278E+01	4.492568657411E+00
C	3.580235628938E-01	2.626645291329E+01	4.165756921313E+00
C	-2.136506831616E-01	2.626501918232E+01	4.164511913333E+00
C	4.227102091610E-01	2.566475474617E+01	4.065600782388E+00
C	-4.277211388075E-01	2.705570333357E+01	4.296977649905E+00
C	-2.782688504124E-01	2.566141356936E+01	4.064218112526E+00
H	-4.278039174556E-01	3.603826022646E+01	5.739532085766E+00
H	4.407137739464E-01	3.481265938323E+01	5.544780124448E+00
H	-2.963641917023E-01	3.481142291279E+01	5.544619989989E+00
H	7.222674881868E-02	3.137647396250E+01	4.997147772760E+00

Z5

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

A	B	C	ALPHA	BETA	GAMMA
16.35099588	500.00000000	500.00000000	90.000000	90.000000	90.000000

ATOMS IN THE ASYMMETRIC UNIT 172 - ATOMS IN THE UNIT CELL: 172

ATOM	X/A	Y(ANGSTROM)	Z(ANGSTROM)
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C	-7.070973266264E-02	3.767146179747E+00	9.882192570777E+00
C	-1.353312724182E-01	4.002491644764E+00	1.044689760811E+01
C	-2.068996686875E-01	4.261226988210E+00	1.107123342395E+01
C	-3.460665541260E-01	5.304515439786E+00	1.359454255337E+01
C	-2.715858522546E-01	4.493829180607E+00	1.163505733422E+01
C	-7.061768785908E-02	2.695407958371E+00	7.269227519905E+00
C	-4.211794461388E-01	5.586985665025E+00	1.424447414675E+01
C	-3.460452333986E-01	4.771809469307E+00	1.228035468288E+01
C	-1.353162581763E-01	2.460535271320E+00	6.706575279707E+00
C	-4.962616024242E-01	5.304759528160E+00	1.359357467824E+01
C	-4.211198423624E-01	4.489978594836E+00	1.162926461027E+01

C -4.962232365461E-01 4.771861915899E+00 1.227941568229E+01
C -4.211002971110E-01 3.959859678329E+00 1.032706668330E+01
C -2.068566465801E-01 2.203594345685E+00 6.081128606672E+00
C -4.211267354777E-01 3.492333233098E+00 9.199254923820E+00
C -2.715883701931E-01 1.970962615993E+00 5.518152887538E+00
C -4.211357261791E-01 2.977518596864E+00 7.949140601214E+00
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C -3.465805660088E-01 1.155146981926E+00 3.554940746871E+00
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H -4.211419182705E-01 4.763308208825E-01 1.923802973194E+00
C 4.299944292916E-01 8.792196609593E-01 2.891900348678E+00
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C 7.884280215190E-02 1.166250050681E+00 3.590986183610E+00
C 7.882064425984E-02 6.990064634732E-01 2.463241410131E+00
C 7.886755804183E-02 1.685506512016E+00 4.839284316807E+00
C 4.292992658167E-01 1.970757918185E+00 5.518021313477E+00
C 2.940575543954E-01 3.810563925465E-01 1.691160935899E+00
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C 7.892616123445E-02 2.151285820939E+00 5.967613326872E+00
C 2.930459911440E-01 2.460589918724E+00 6.707145255417E+00
C 7.889177027457E-02 2.696162817669E+00 7.263621601290E+00
C 2.284020383282E-01 2.695213498584E+00 7.271531996633E+00
C 2.289880351898E-01 1.528979151088E-01 1.139989621490E+00
C 3.790817324836E-03 2.955571519703E+00 7.923228764668E+00
C 1.539553789612E-01 2.955368467941E+00 7.924381565439E+00
C 7.883532606645E-02 1.617846967720E-01 1.161982025117E+00
C 3.752522536800E-03 3.507634612300E+00 9.229276739549E+00
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C 1.539237668133E-01 3.507762365660E+00 9.230338456741E+00
C 7.882160397273E-02 3.767371403007E+00 9.889595881183E+00
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C 5.183296157091E-03 -6.467908439500E-01 -7.987413517926E-01
C 4.293589879817E-01 4.493636550366E+00 1.163313676496E+01
C 7.887279504759E-02 -9.100024792967E-01 -1.436135403860E+00
H 2.103387536414E-01 -8.508215348232E-01 -1.291566687191E+00
H -5.259663805375E-02 -8.502525097895E-01 -1.292928681299E+00
H 7.888805420333E-02 -1.324406372495E+00 -2.440049004727E+00

C 3.770999891888E-03 6.566030141721E+00 1.664554562148E+01
C 3.737882673535E-03 7.116096526294E+00 1.795242036951E+01
C 7.879250412298E-02 4.312487984620E+00 1.118522899800E+01
C 7.888046067173E-02 4.778807010230E+00 1.231358267118E+01
C 7.890135890045E-02 5.298834097152E+00 1.356090786609E+01
C 7.892565217765E-02 5.764166148446E+00 1.468966418704E+01
C 7.889317107050E-02 6.307877373710E+00 1.598571022377E+01
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C 7.881446944008E-02 7.374605889545E+00 1.861331169447E+01
C 1.539781670276E-01 6.566483231021E+00 1.664656059858E+01
C 1.539322573787E-01 7.116396751115E+00 1.795356310352E+01
C -1.353507349332E-01 7.609495118815E+00 1.917027640156E+01
C -7.066784656066E-02 6.306300535176E+00 1.599197379742E+01
C 2.284424754282E-01 6.307686707839E+00 1.599366863832E+01
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C -2.069064965791E-01 7.867683951209E+00 1.979491602458E+01
C 2.930469889757E-01 7.610475039588E+00 1.917040358836E+01
C -2.715646537663E-01 8.100042604630E+00 2.035982401858E+01
C 2.930418787982E-01 6.072825648204E+00 1.542790970113E+01
C -3.460693314612E-01 8.907651573493E+00 2.232023753995E+01
C -1.353646065341E-01 6.072162014983E+00 1.542894660496E+01
C -3.460266316819E-01 8.377096776346E+00 2.100521175426E+01
C -4.211897368286E-01 9.189188580957E+00 2.297056700483E+01
C 3.646222704163E-01 7.868449862828E+00 1.979488100200E+01
C -4.962690743544E-01 8.907519812158E+00 2.231930321671E+01
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C 4.293660127097E-01 8.100061387687E+00 2.035742463159E+01
C -4.962173128054E-01 8.376989266264E+00 2.100425724020E+01
C 3.645995545385E-01 5.814552395811E+00 1.480317997282E+01
C -4.210752968808E-01 7.565585463517E+00 1.905203004235E+01
C -4.210865000338E-01 7.098157812094E+00 1.792399043543E+01
C 4.292783833021E-01 5.582354762131E+00 1.423893604041E+01
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C -4.211173688615E-01 6.585069382803E+00 1.667416653104E+01
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C -4.211186701021E-01 1.069590279769E+01 2.665165010729E+01
C -4.211794214813E-01 9.716082327427E+00 2.427364193040E+01
C -4.210903612125E-01 1.115893089274E+01 2.778145442895E+01
C -2.716400475747E-01 9.184697644436E+00 2.296657469984E+01
C -4.211421168278E-01 1.170302890566E+01 2.907768906399E+01
C -2.069771907107E-01 9.415728771864E+00 2.353201427448E+01
C 4.292393032377E-01 9.184001883018E+00 2.296415019610E+01
C -3.460685851959E-01 1.196253190845E+01 2.973803336235E+01
C -4.962322741290E-01 1.196289756452E+01 2.973706851296E+01
C -2.716049822550E-01 1.170147096153E+01 2.908582626928E+01
C 4.293094953164E-01 1.170260818771E+01 2.908419919491E+01
C 3.645873015367E-01 9.415817851409E+00 2.352965240603E+01

C	3.646242397952E-01	1.146924663245E+01	2.852053904004E+01
C	-2.069631248209E-01	1.146630028452E+01	2.852154149555E+01
C	-1.353875165327E-01	9.673151597815E+00	2.415614652397E+01
C	-3.460878470649E-01	1.251449226249E+01	3.104420281221E+01
C	-4.962483644405E-01	1.251468920638E+01	3.104330201309E+01
C	2.930348095995E-01	9.673100851112E+00	2.415468267303E+01
C	-4.211811242713E-01	1.277388483994E+01	3.170402309624E+01
C	2.930694635231E-01	1.121380401776E+01	2.789503585899E+01
C	-1.353950656392E-01	1.121109384148E+01	2.789581067006E+01
C	-4.211503848029E-01	1.636043374726E+01	4.041149380585E+01
C	4.293138802165E-01	1.277512782184E+01	3.169609852666E+01
C	-2.716557396832E-01	1.277531666172E+01	3.169736810242E+01
C	-4.948341552220E-01	1.609925184707E+01	3.977306505669E+01
C	2.283991019525E-01	9.906827477673E+00	2.471971344888E+01
C	-7.069567404837E-02	9.907281676286E+00	2.471940128365E+01
C	-4.212178240858E-01	1.331741796321E+01	3.300051471498E+01
C	-3.474737897834E-01	1.609876109843E+01	3.977304848521E+01
C	2.283516819907E-01	1.097743943564E+01	2.733369633893E+01
C	-4.960545458784E-01	1.556833203554E+01	3.847640513973E+01
C	3.646547307604E-01	1.300942563643E+01	3.226024715732E+01
C	-7.071243828121E-02	1.097659029868E+01	2.733238464319E+01
C	-4.212151116198E-01	1.378092290357E+01	3.412983715920E+01
C	-2.069954194492E-01	1.300925479518E+01	3.226146469248E+01
C	-3.462660609750E-01	1.556777466260E+01	3.847643790020E+01
C	-4.211630569573E-01	1.529519059141E+01	3.781074235524E+01
C	4.286829636846E-01	1.530454687530E+01	3.783341803319E+01
C	-4.212072333938E-01	1.429731962533E+01	3.537905248994E+01
C	-4.211724296108E-01	1.476147753203E+01	3.650813804213E+01
C	1.539517856544E-01	1.016569944920E+01	2.537353153172E+01
C	3.636352097046E-01	1.507753619129E+01	3.728116750961E+01
C	1.539285286442E-01	1.071632524660E+01	2.668027106214E+01
C	-2.710074757079E-01	1.530384896973E+01	3.783340377039E+01
C	2.931212993639E-01	1.326587536808E+01	3.288612846306E+01
C	-2.059396374638E-01	1.507700723227E+01	3.728175600830E+01
C	-1.354651945076E-01	1.326602079680E+01	3.288670496055E+01
C	7.885766388368E-02	9.906541711527E+00	2.471329045489E+01
C	2.918703994142E-01	1.481987812820E+01	3.665463615123E+01
C	7.886897155923E-02	9.363360098686E+00	2.341690229782E+01
C	7.883151000574E-02	8.899254870309E+00	2.228756317402E+01
C	7.882233079940E-02	1.097522160432E+01	2.734010871381E+01
C	2.283924974910E-01	1.349835337520E+01	3.344929842986E+01
C	2.277192022585E-01	1.458281101391E+01	3.607856134066E+01
C	-1.341700456114E-01	1.481932993934E+01	3.665531231390E+01
C	7.880683539221E-02	1.151791664883E+01	2.863700234272E+01
C	7.883061571075E-02	8.381151845430E+00	2.103933415963E+01
C	-7.073041018678E-02	1.349860310284E+01	3.344950913801E+01
C	3.753919166392E-03	1.016578081286E+01	2.537293199392E+01
H	-4.211447993727E-01	1.677177388277E+01	4.141666676453E+01
C	3.741143923784E-03	1.071605141709E+01	2.667976771210E+01

C	7.884991841210E-02	1.198184477856E+01	2.976620276786E+01
H	4.473811017195E-01	1.630136397332E+01	4.026766352459E+01
C	7.877290400246E-02	7.916873142784E+00	1.991000812998E+01
C	1.540099547431E-01	1.376786132618E+01	3.409962833039E+01
C	1.534133427870E-01	1.430940716041E+01	3.541454984294E+01
C	-7.002195903538E-02	1.458230616624E+01	3.607913372096E+01
H	-2.896833153723E-01	1.630065704575E+01	4.026756232277E+01
C	7.886151057489E-02	1.249873830602E+01	3.101571373441E+01
C	7.884955888963E-02	1.296376161253E+01	3.214418443098E+01
C	7.883721099944E-02	1.349914325580E+01	3.344679006541E+01
C	7.884684421411E-02	1.456919490784E+01	3.604544926079E+01
C	3.668258203000E-03	1.376781059092E+01	3.409969065480E+01
C	4.277901815042E-03	1.430906387881E+01	3.541482043473E+01
H	7.885042277224E-02	1.498219215904E+01	3.704821169087E+01

Table S4: Band gaps of A(n)- and Z(n)-GDYNRs of different widths computed at PBE0/6-31G(d) and HSE06/6-31G(d) level of theory

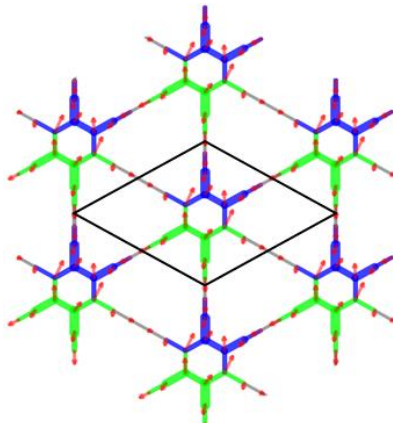
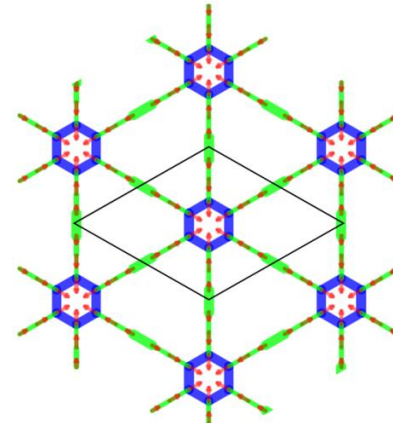
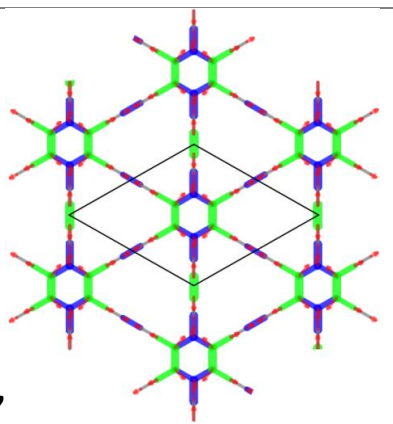
NR	Band Gap PBE0 (eV)	Band Gap HSE06 (eV)
A1	2.836	2.2248
A2	2.281	1.7159
A3	2.014	1.4797
A4	1.883	1.3588
A5	1.804	1.2882
Z1	3.933	3.2814
Z1.5	2.866	2.2919
Z2	2.410	1.8702
Z2.5	2.173	1.6492
Z3	2.030	1.5146
Z3.5	1.937	1.4259
Z4	1.873	1.3636
Z4.5	1.826	1.3181
Z5	1.791	/

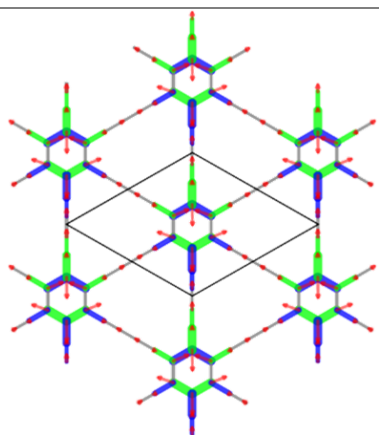
Table S5: DFT computed [PBE0/6-31G(d)] values of vibrational frequency (cm^{-1}), IR intensity (km/mol) and Raman activity ($\text{\AA}^4/\text{amu}$) of 2D-GDY. It should be noted that there are two modes with large imaginary frequency values (-388 and -96 cm^{-1}) in this Table. The occurrence of imaginary frequencies associated to out-of-plane displacements of carbon atoms in arenes such as the GDY systems investigated in this work is a spurious computational effect related with the incompleteness of the atomic orbital basis set [H. Torii et al. J. Mol. Struct. - Theochem 500, 311 (2000), D. Moran et al. J. Am. Chem. Soc. 128, 9342 (2006), D. Asturiol et al. J. Chem. Phys. 128, 144108 (2008)]. It is not expected to affect the in-plane vibrational structure.

Wavenumber (cm^{-1})	Symmetry species	IR intensity [km/mol]	Raman activity [$\text{\AA}^4/\text{amu}$]
-388	B _{2g}	0	0
-96	B _{2u}	0	0
-10	A _{2u}	0	0
-3	E _{1u}	0	0
17	E _{1u}	0	0
87	A _{2g}	0	0
96	E _{2u}	0	0
96	E _{2u}	0	0
137	E _{1g}	0	5
137	E _{1g}	0	5
172	E _{1u}	0.3	0
172	E _{1u}	0.3	0
183	A _{2u}	0.1	0
307	B _{2g}	0	0
392	E _{2u}	0	0
392	E _{2u}	0	0
396	E _{2g}	0	973
396	E _{2g}	0	973
410	B _{2u}	0	0
418	E _{1u}	6	0
418	E _{1u}	6	0
474	E _{1g}	0	40
474	E _{1g}	0	40
485	A _{2u}	0.2	0
485	A _{2g}	0	0
504	B _{1u}	0	0
573	E _{2g}	0	740
573	E _{2g}	0	740
583	E _{2u}	0	0
583	E _{2u}	0	0
640	B _{2g}	0	0
652	E _{1g}	0	393
652	E _{1g}	0	393
696	A _{2g}	0	0
790	E _{2g}	0	2673
790	E _{2g}	0	2673
893	E _{1u}	6.7	0
893	E _{1u}	6.7	0
983	A _{1g}	0	231213
1317	B _{2u}	0	0
1342	B _{1u}	0	0
1382	E _{2g}	0	6285
1382	E _{2g}	0	6285
1429	E _{1u}	522	0
1429	E _{1u}	522	0
1490	A _{1g}	0	869870
1573	E _{2g}	0	248915
1573	E _{2g}	0	248915
2267	E _{1u}	240	0
2267	E _{1u}	240	0
2276	A _{1g}	0	3707443
2282	B _{1u}	0	0
2335	E _{2g}	0	638183
2335	E _{2g}	0	638183

Table S6: Sketches of DFT computed [PBE0/6-31G(d)] Raman and IR active normal modes of 2D-GDY.

Red arrows indicate atomic displacements while green and blue colors indicate the active bond stretching vibrations in each normal mode. The different colors indicate different phases of the vibration, while the line width is proportional to its amplitude.

Normal Mode	Frequency (cm ⁻¹)	Symmetry species	IR intensity (km/mol)	Raman activity (A ⁴ /amu)
<p>R'</p> 	893	E _{1u}	7	0
<p>B</p> 	983	A _{1g}	0	231213
<p>G'</p> 	1382	E _{2g}	0	6285



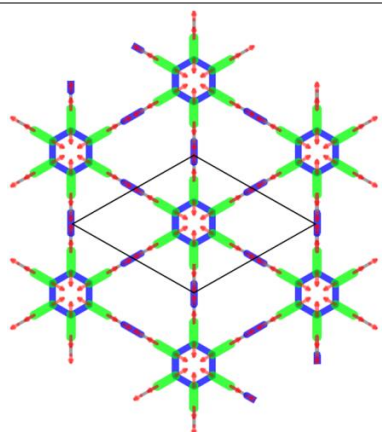
1429

E_{1u}

522

0

R



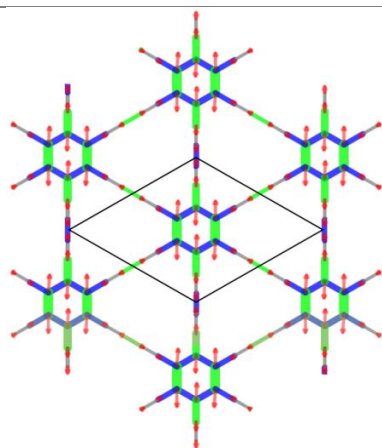
1490

A_{1g}

0

869870

D



1573

E_{2g}

0

248915

G

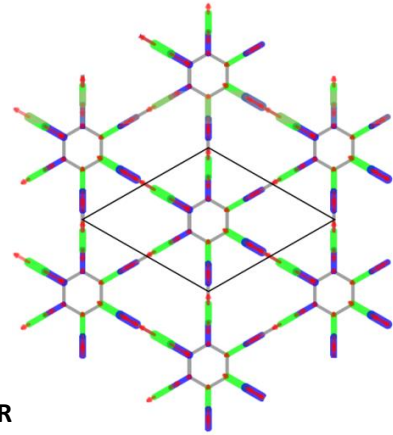
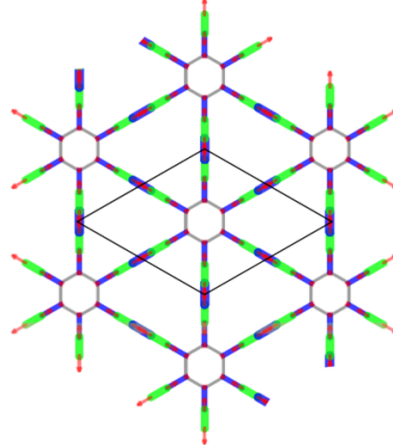
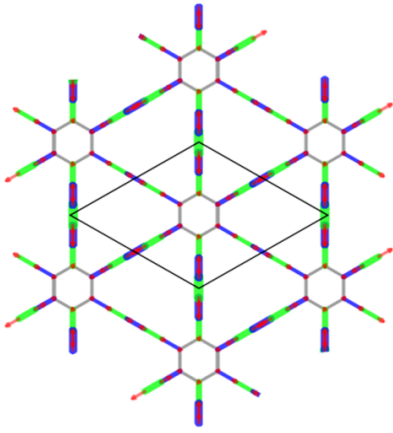
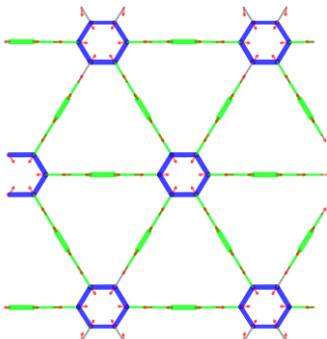
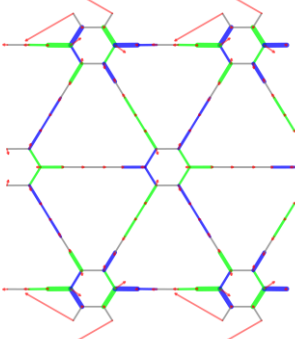
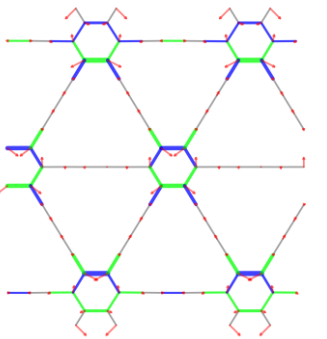
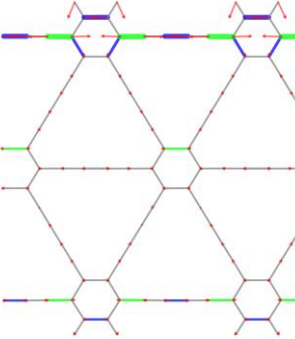
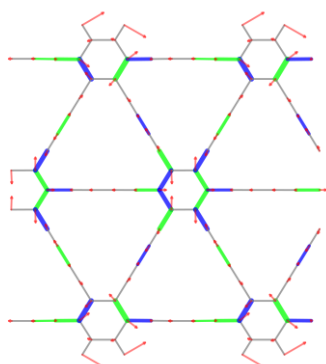
γ_{IR}		2267	E_{1u}	240	0
γ		2276	A_{1g}	0	3707443
γ'		2335	E_{2g}	0	638183

Table S7: Sketches of DFT computed [PBE0/6-31G(d)] Raman active normal modes of A(n)- and (Z(n)- GDYNR.

Red arrows indicate atomic displacements while green and blue colors indicate the active bond stretching vibrations in each normal mode. The different colors indicate different phases of the vibration, while the line width is proportional to its amplitude.

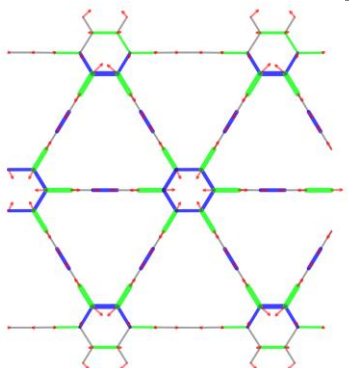
Normal modes A3	Frequency [cm ⁻¹]	Raman activity [A ⁴ /amu]	IR Intensity [km/mol]
	990	179315	0
	1266	1	86
	1433	0	172
	1452	157137	1



1469

9

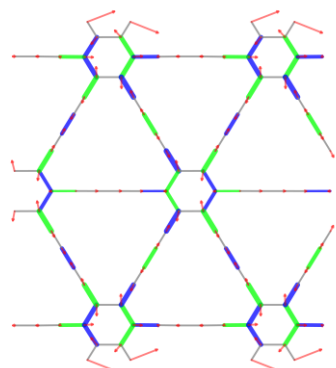
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1499

373617

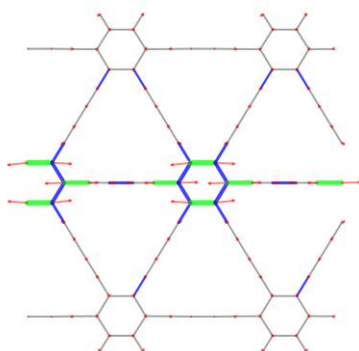
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1519

40

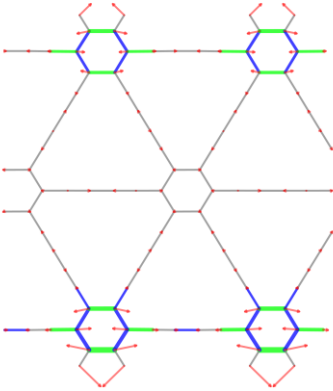
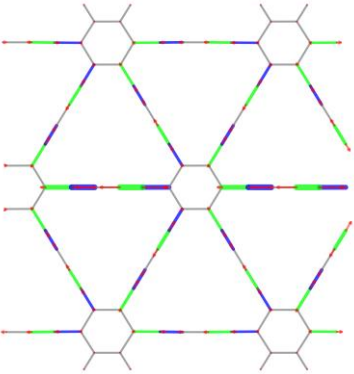
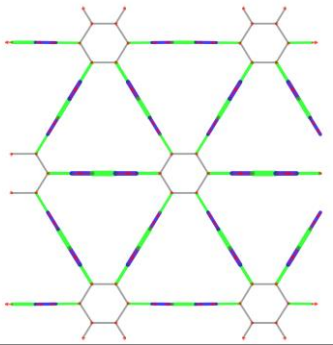
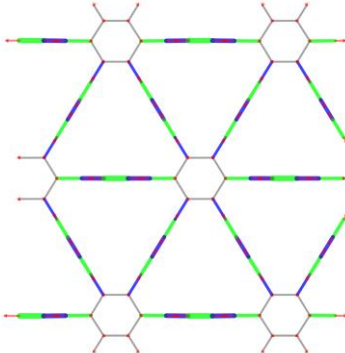
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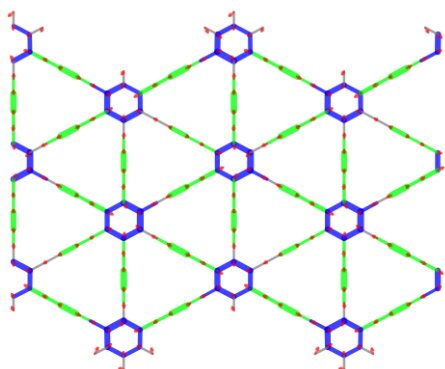


1571

212736

0

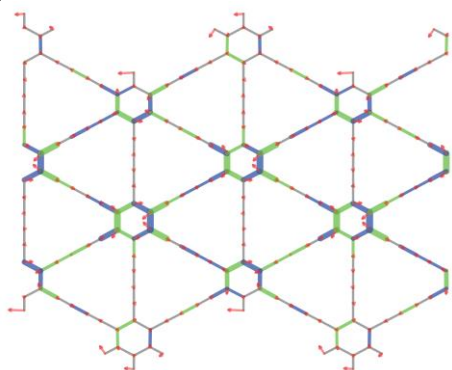
	1630	609858	0
	2270	7	322
	2293	2763591	0
	2342	1592954	0
Normal modes Z3	Frequency [cm⁻¹]	Raman activity [A⁴/amu]	IR Intensity [km/mol]



990

265254

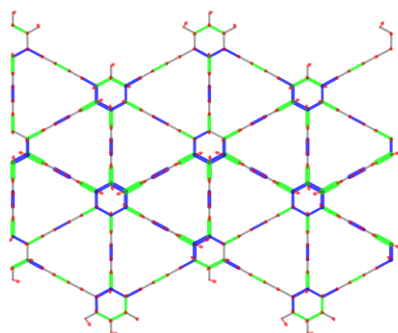
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1448

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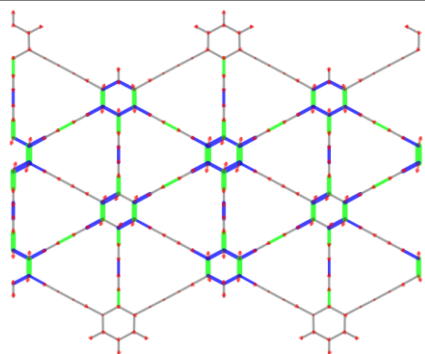
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1498

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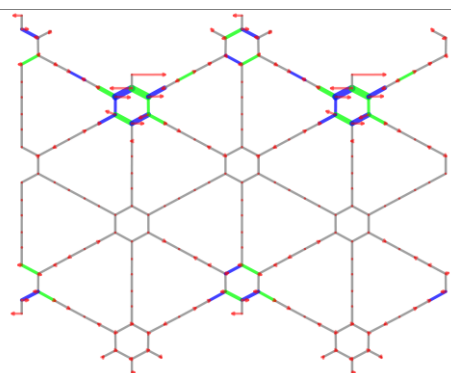
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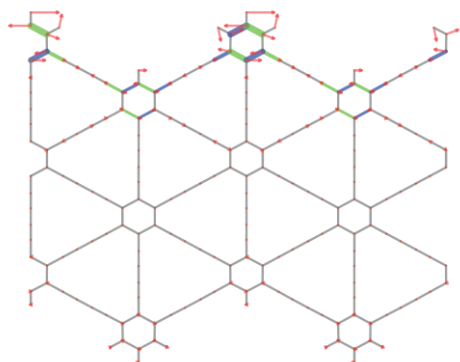
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1619

63719

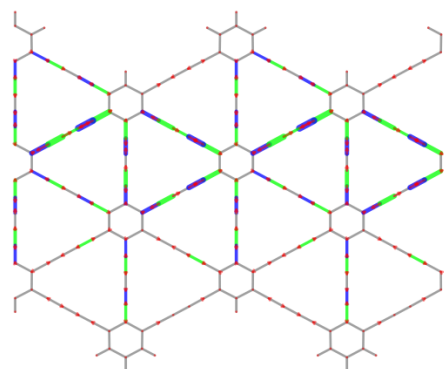
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1627

9775

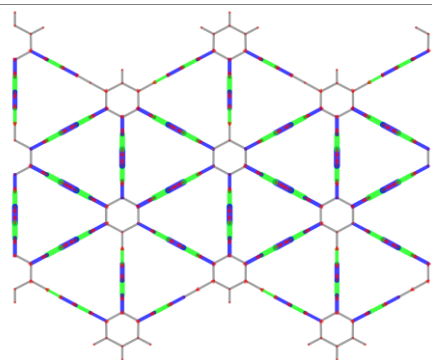
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2269

13163

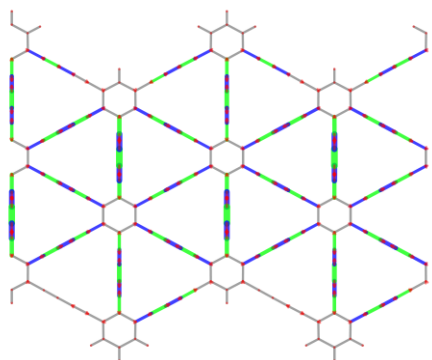
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2292

4984467

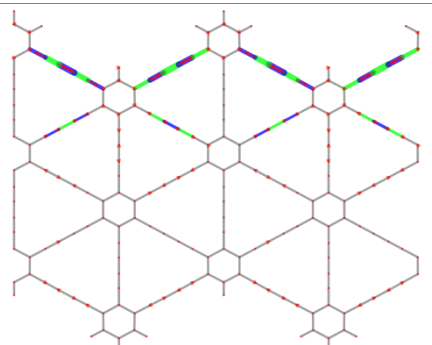
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2347

988883

0



2350

110847

97

Table S8: DFT computed [PBE0/6-31G(d)] values of vibrational frequency (cm^{-1}), IR intensity (km/mol) and Raman activity (A^4/amu) of the diphenyl-polyynes with 4 sp-carbon atoms.

Frequency (cm^{-1})	Symmetry species	IR intensity [km/mol]	Raman activity [A^4/amu]
7	A _u	0	0
29	B _{1u}	0.56	0
34	B _{2u}	0.8	0
79	B _{2g}	0	5.77
96	B _{1g}	0	4.28
190	B _{2u}	0.0	0
208	B _{1u}	0.04	0
233	A _g	0	0.13
315	B _{1g}	0	15.11
402	B _{2u}	0.43	0
412	A _u	0	0
413	B _{3g}	0	0.01
463	B _{2g}	0	0.21
475	B _{3u}	18.79	0
511	B _{1u}	1.75	0
520	B _{1g}	0	3.12
553	B _{2u}	7.29	0
560	B _{2g}	0	33.5
633	B _{1u}	0.0	0
634	B _{2g}	0	4.71
663	B _{1g}	0	106.41
677	A _g	0	43.99
707	B _{1g}	0	8.74
708	B _{2u}	32.88	0
776	B _{2u}	62.03	0
777	B _{1g}	0	2.78
788	B _{3u}	8.21	0
864	A _u	0	0
864	B _{3g}	0	15.47
938	B _{2u}	4.71	0
938	B _{1g}	0	12.85
985	A _u	0	0
985	B _{3g}	0	0.12
1010	B _{1g}	0	4.55
1010	B _{2u}	0.07	0
1011	A _g	0	69.03
1018	B _{3u}	3.41	0
1024	A _g	0	1012.84
1067	B _{3u}	5.34	0
1071	A _g	0	27.77
1116	B _{2g}	0	0.39
1116	B _{1u}	6.28	0

1188	B _{1u}	0.01	0
1188	B _{2g}	0	34.48
1206	B _{3u}	1.9	0
1208	A _g	0	207.7
1254	B _{3u}	7.68	0
1336	B _{1u}	0.18	0
1336	B _{2g}	0	0.52
1384	B _{2g}	0	54.58
1384	B _{1u}	0.51	0
1408	A _g	0	728.46
1495	B _{2g}	0	50.06
1495	B _{1u}	10.55	0
1544	B _{3u}	42.17	0
1561	A _g	0	968.32
1654	B _{1u}	1.47	0
1654	B _{2g}	0	0.26
1687	B _{3u}	18.24	0
1688	A _g	0	4480.41
2282	B _{3u}	0.15	0
2369	A _g	0	29522.21
3203	B _{3u}	6.15	0
3203	A _g	0	57.54
3212	B _{2g}	0	356.23
3212	B _{1u}	13.21	0
3224	B _{3u}	45.33	0
3224	A _g	0	479.01
3232	B _{2g}	0	19.34
3232	B _{1u}	41.15	0
3236	B _{3u}	30.96	0
3236	A _g	0	668.23

Table S9: Sketches of DFT computed [PBE0/6-31G(d)] relevant normal modes of the diphenyl-polyynes with 4 sp-carbon atoms ; the two different colors indicate stretching of the bonds with different phases

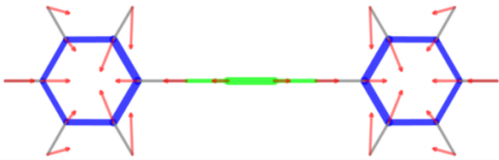
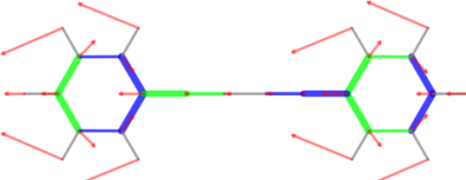
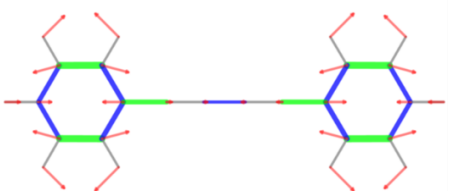

Normal modes	Frequency [cm ⁻¹]	Symmetry species	IR intensity [km/mol]	Raman activity [A ⁴ /amu]
	1024	A _g	0	1013
	1561	A _g	0	968
	1688	A _g	0	4480
	2369	A _g	0	29522

Table S10: DFT computed [PBE0/6-31G(d)] Raman polarizability tensors associated to the most relevant Raman transitions of 2D-GDY

Symmetry species	Frequency (cm^{-1})	Raman activity ($\text{Å}^4/\text{amu}$)	$d\alpha_{xx}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)	$d\alpha_{xy}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)	$d\alpha_{yy}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)	$d\alpha_{xz}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)	$d\alpha_{yz}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)	$d\alpha_{zz}/dq$ ($\text{Å}^2/\sqrt{\text{amu}}$)
A1g	983	231213	93	0	93	0	0	0.0
E2g	1382	12571	-17	0	17	0	0	0.0
			0	17	0	0	0	0.0
A1g	1490	869870	179	0	179	0	0	0.0
E2g	1573	497834	109	0	-109	0	0	0.0
			0	-109	0	0	0	0.0
A1g	2276	3707443	371	0	371	0	0	0.0
E2g	2335	1276368	174	0	-174	0	0	0.0
			0	-174	0	0	0	0.0

Table S11: DFT computed [PBE0/6-31G(d)] dipole derivatives associated to the most relevant IR transitions of 2D-GDY

Symmetry Species	Frequency (cm^{-1})	IR Intensity (km/mol)	$d\mu_x/dq$ (debye/($\text{Å} * \sqrt{\text{amu}}$))	$d\mu_y/dq$ (debye/($\text{Å} * \sqrt{\text{amu}}$))	$d\mu_z/dq$ (debye/($\text{Å} * \sqrt{\text{amu}}$))
E1u	893	13	0	0.4	0
E1u	1429	1044	0	-3.5	0
E1u	2267	480	-2.4	0	0

Table S12: DFT computed [PBE0/6-31G(d)] Raman polarizability tensors associated to the most relevant Raman transitions of A3-GDYNR. The phonons are classified according to the D_{2h} symmetry group. In the last column, the ratio between yy and xx components highlights the strong anisotropy of the Raman tensors: one only element (xx), where x is the crystal axis direction, is relevant.

Symmetry	Frequency (cm^{-1})	Raman activity (A^4/amu)	$d\alpha_{xx}/dq$ (A^2/\sqrt{amu})	$d\alpha_{xy}/dq$ (A^2/\sqrt{amu})	$d\alpha_{yy}/dq$ (A^2/\sqrt{amu})	$d\alpha_{xz}/dq$ (A^2/\sqrt{amu})	$d\alpha_{yz}/dq$ (A^2/\sqrt{amu})	$d\alpha_{zz}/dq$ (A^2/\sqrt{amu})	$\frac{(d\alpha_{yy}/dq)}{(d\alpha_{xx}/dq)}$
Ag	990	179315	-119	0	-17	0	0	0.0	0.14
Ag	1452	157137	91	0	4	0	0	0.0	0.04
Ag	1499	373617	170	0	31	0	0	0.0	0.18
Ag	1571	212736	134	0	-17	0	0	0.0	-0.13
Ag	1630	609858	-217	0	3	0	0	0.0	-0.01
Ag	2293	2763591	468	0	64	0	0	-0.1	0.14
Ag	2342	1592954	367	0	-33	0	0	0.0	-0.09

Table S13: DFT computed [PBE0/6-31G(d)] dipole derivatives associated to the most relevant IR transitions of A3-GDYNR. The phonons are classified according to the D_{2h} symmetry group.

Symmetry	Frequency (cm^{-1})	IR Intensity (km/mol)	$d\mu_x/dq$ (debye/($A * \sqrt{amu}$))	$d\mu_y/dq$ (debye/($A * \sqrt{amu}$))	$d\mu_z/dq$ (debye/($A * \sqrt{amu}$))
B3u	1266	86	-1,4	0.0	0.0
B2u	1433	172	0,0	-2.0	0.0
B3u	1469	796	4,3	0.0	0.0
B3u	1519	113	1,6	0.0	0.0
B3u	2270	322	2,8	0.1	0.0

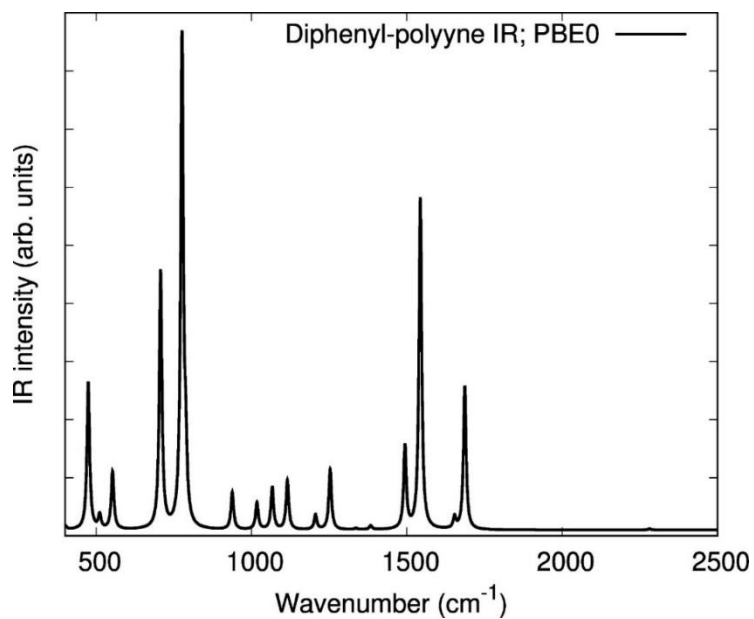


Figure S1: DFT computed [PBE0/6-31G(d)] IR spectrum of the diphenyl-polyynes with 4 sp-carbon atoms

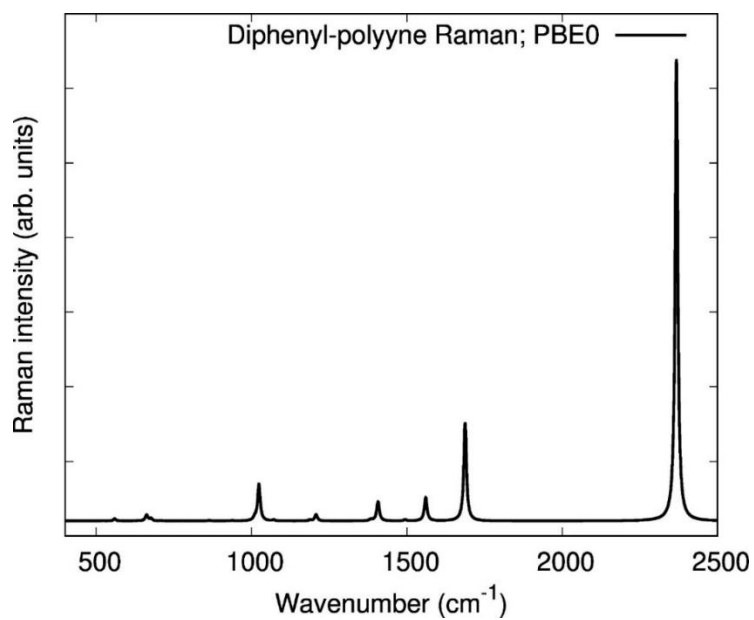


Figure S2: DFT computed [PBE0/6-31G(d)] Raman spectrum of the diphenyl-polyynes with 4 sp-carbon atoms

Spectroscopic marker bands of armchair and zigzag GDYNR.

In Figure S3 we directly compare the Raman and IR spectra of A(3)-GDYNR and Z(*n*)-GDYNR (*n* = 2.5, 3) with those of 2D-GDY in order to reveal the peculiar marker bands of A- and Z- GDYNR.

As mentioned in the paper, while in the Raman spectra Z-edges do not show intense marker bands, A(3)-GDYNR presents a relevant marker bands at 1630 cm⁻¹, which can be considered not only as a marker of confinement, but also a reliable marker of the presence A edges.

By comparing the Raman spectra of integer and half integer Z(*n*)-GDYNRs, we can notice small but clear differences. For instance, Z(3) shows one only band originated by the superposition of two normal modes located at 1490 cm⁻¹ and at 1498 cm⁻¹ while for Z(2.5), in the same spectral range, two individual components are computed, located at 1482 cm⁻¹ and at 1503 cm⁻¹ respectively, giving rise to a doublet of peaks. However, these bands find a clear correspondence with D line of 2D crystal and cannot be taken as marker band of the ribbons.

Considering the IR spectrum, a reliable marker of Z(*n*)-GDYNRs can be found in the extra band predicted at about 2350 cm⁻¹, which does not appear in the case of for A(*n*)-GDYNRs. In addition, another marker of Z edge is the band at about 1620 cm⁻¹. On the other hand, A(*n*)-GDNRs display several marker bands at about 1270 and 1405 cm⁻¹.

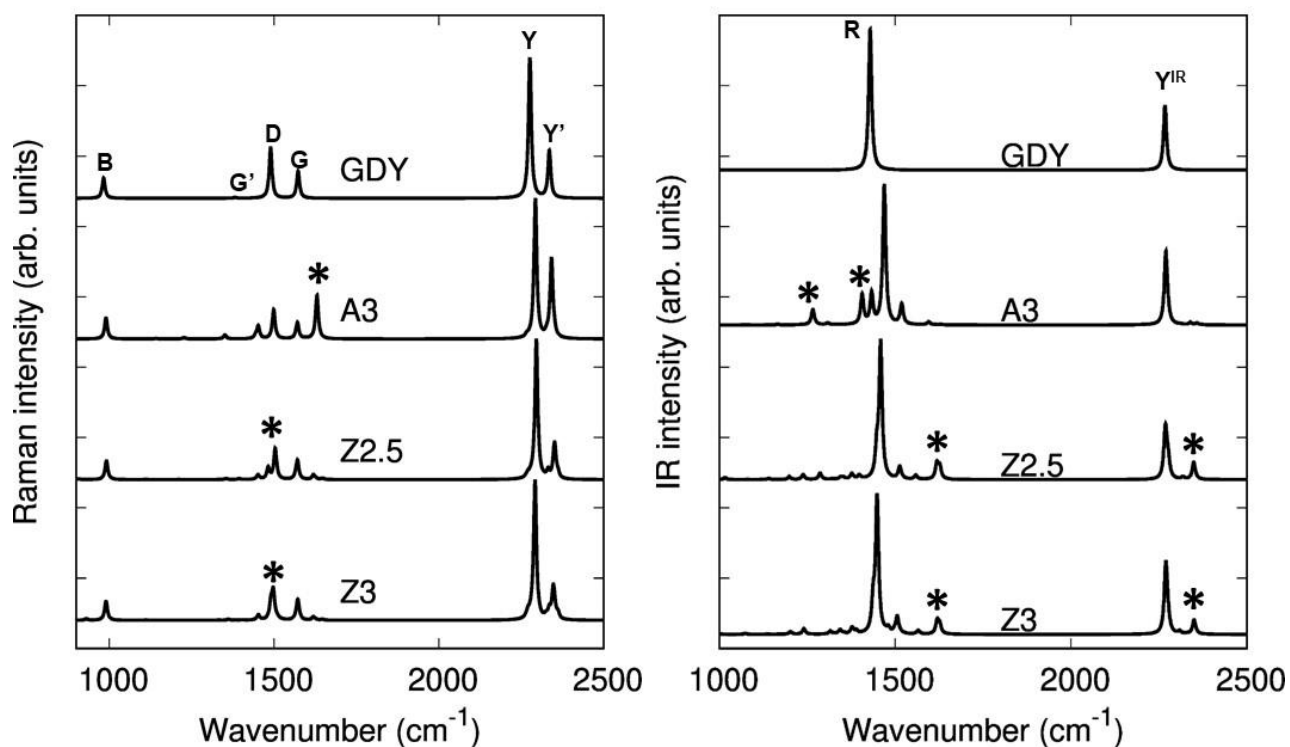


Figure S3: Comparison among the DFT computed (PBE0/6-31G(d)) Raman and IR spectra of 2D-GDY, with GDYNRs having different edges and the same width. The wavenumber values are not scaled. The bands discussed in the text are marked by *.