Computational study of NMR chemical shifts in periodic graphane-based systems

Master's thesis

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1. Introduction

Graphene, a material consisting of a single layer of carbon atoms in a hexagonal lattice, theoretically predicted in 1947 [1] and first synthesized in 2004 [2], is a significant material in nanoscience and nanotechnology today [3]. This is explained by its extraordinary properties. It is the strongest material ever tested – 200 times stronger than steel. Also, it is the best material for conducting electricity and heat [4]. Recent experimental studies also show that graphene systems can be tuned to become correlated insulators or superconductors [5, 6]. To no surprise it has a lot of different potential uses and applications. Examples of these would be its usage in composite materials [7], electronics [8] or in quantum dots [9].

The properties of graphene can also be tuned by functionalization. For example the material can be hydrogenated, thus creating hydrographene which is also known as graphane [10, 11]. Graphene is originally a zero band-gap semiconductor [4], but after the hydrogenation process it becomes an insulator with a band gap [12]. Varying the degree of hydrogenation, it is possible to tune its electronic properties to a desired point [13]. Other possible applications for graphane are for example hydrogen storage [14] and lithium-ion batteries [15].

In the hydrogenation process it is possible for the hydrogen atoms to attach to the graphane sheet on either side. This allows graphane to have multiple conformations. Six of them were studied in this work. Their naming conventions differ in literature but the ones used here are chair [14, 16], boat-1 [14, 16, 17], boat-2 [17, 18], stirrup [16, 17, 19], twistboat [20] and tricycle [21] conformations.

There are various methods for producing graphene-based carbon nanomaterials. In the case of graphane, a so-called Birch reduction can be used [22, 23]. Vishnyakova *et al.* [22, 23] used it to produce graphane from commercial graphite, using Li/NH_3 as the reducing agent and tert-butyl alcohol as the proton source. The resulting product was analyzed to be certain of its structure and composition.

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful experimental tool for studying chemical, dynamical and spatial properties of different materials. It is based on a phenomenon called nuclear magnetic resonance. It occurs when NMR active nuclei are affected by a static external magnetic field and an oscillating external magnetic field [24]. NMR spectroscopy is used widely for different purposes in various fields of research [25]. In chemistry it is used for chemical analysis and studying structures of molecules. NMR can also be used to investigate orientation, rotation and diffusion of molecules. In medicine, and also in materials science, NMR is used in magnetic resonance imaging

(MRI). MRI is especially useful because NMR is based on radio-frequency pulses that are not harmful for living specimens as their frequency is around 10 to 800 MHz [26]. This is a useful feature also in other fields of research where it is beneficial not to harm the investigated sample.

It is possible to interpret results from a NMR experiment (usually in the form of spectra) empirically but sometimes it is hard or even impossible. Computational NMR can be used to calculate desired NMR parameters such as chemical shift from first principles. For instance in the study made by Vishnyakova *et al.* [22,23] the produced graphane was analyzed with solid-state $^{13}\mathrm{C}$ NMR spectroscopy and the results were compared to a computational NMR study made by Vähäkangas *et al.* [27]. Based on the comparison they were able to conclude that there appear to be interior benzene rings surrounded by fully hydrogenated graphene. However in this case a more thorough computational study would be desirable as the chair conformation is the only one with computed values of NMR chemical shifts and clearly other conformations are also possible [21].

The aim of this study is to provide comprehensive computational NMR chemical shifts for graphane using the periodic GIPAW method [28]. These computed values can then be used for example to assist the analysis of experimental NMR spectra. Values of $^{13}\mathrm{C}$ and $^{1}\mathrm{H}$ NMR chemical shifts are calculated for the chair, boat-1, boat-2, stirrup, twistboat and tricycle conformations of graphane in 1-, 2-, 3-layered and bulk systems. In addition, graphene-defected 1-layer conformations of graphane are investigated.

2. Theory

In this chapter the theory for the computation of NMR parameters in periodic graphene-based systems is presented. First, we will take a look at the basics of NMR spectroscopy in general. After that we will discuss the theory behind computational NMR. In this case the important frameworks for the used theory are the Density Functional Theory (DFT) [29] and the Gauge-Including Projector Augmented Wave Method (GIPAW) [28].

2.1. NMR spectroscopy

The nuclear magnetic resonance phenomenon rises from the interaction between an external magnetic field and a NMR active nucleus, which possesses a non-zero nuclear spin and therefore a magnetic moment, $\boldsymbol{m}_K = \gamma_K \hbar \boldsymbol{I}_K$, where γ_K is the gyromagnetic ratio of the nucleus K, $\hbar$ is the reduced Planck constant and $\boldsymbol{I}_K$ is the spin operator of the nucleus K [25]. For example, for a $^{13}\mathrm{C}$ nucleus, the quantum number related to the length of the $\boldsymbol{I}_K$ vector is $I_K = 1/2$. Due to the so-called Zeeman effect, the external magnetic field splits the energy levels of a nucleus as shown in Figure 2.1 [30]. The energy of the nucleus can be written as

$$E_m = -\gamma \hbar B_z m \tag{2.1}$$

where m is the magnetic quantum number, which can have values between $-I_K$ and I_K in integer steps.

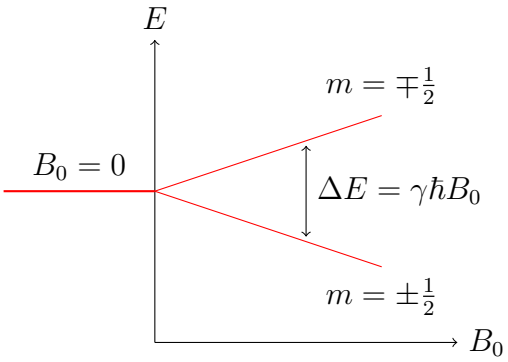

Figure 2.1: An external magnetic field $\boldsymbol{B}_0$ splits the energy levels of an NMR active spin-1/2 nucleus.

The allowed transitions between energy levels are those where $\Delta m = \pm 1$. The energy difference in an allowed transition is therefore

$$|\Delta E| = \gamma \hbar B_0 \tag{2.2}$$

and the frequency of the emitted or absorbed photon is

$$\nu = \frac{|\Delta E|}{h} = \frac{\gamma}{2\pi} B_0. \tag{2.3}$$

This frequency ν is commonly known as the Larmor frequency.

2.1.1. Nuclear spin Hamiltonian

The surroundings of the NMR active nucleus cause small but significant changes in the magnetic field experienced by the nucleus. This enables us to gain valuable chemical and physical information about the investigated system. The NMR spectrum can be reproduced using an effective nuclear spin Hamiltonian (expressed generally in unit of E/h) [31]:

$$\hat{H}^{\text{NMR}} = -\frac{1}{2\pi} \sum_{K=1}^{N} \gamma_K \boldsymbol{B}_0 \cdot (\mathbf{1} - \boldsymbol{\sigma}_K) \cdot \boldsymbol{I}_K + \frac{1}{2} \sum_{K,L=1}^{N} \boldsymbol{I}_K \cdot (\boldsymbol{D}_{KL} + \boldsymbol{J}_{KL}) \cdot \boldsymbol{I}_L. \tag{2.4}$$

The first term in Equation (2.4) describes the NMR shielding caused by the electrons nearby the nucleus K [31]. In the Hamiltonian, $\boldsymbol{\sigma}_K$ is the shielding tensor, $\boldsymbol{I}_K$ is the nuclear spin operator, $\mathbf{1}$ is the 3×3 unit tensor, $\boldsymbol{B}_0$ is the external magnetic field and γ_K is the gyromagnetic ratio of the nucleus K.

The second term in the $\hat{H}^{\text{NMR}}$ describes the direct dipolar and indirect spin-spin couplings [31]. Both couplings are caused by the spin magnetic moments of the nuclei. In the direct dipolar coupling, the small magnetic field caused by the spin magnetic moment of nucleus K affects the magnetic field experienced by nucleus L and vice versa. This interaction is described by the direct dipolar coupling tensor $\boldsymbol{D}_{KL}$ The direct dipolar coupling cannot be detected in isotropic fluids because due to isotropic movement of the molecules it will average out to zero, *i.e.*, it is an anisotropic interaction. The trace of $\boldsymbol{D}_{KL}$ is zero [30].

However, the indirect spin-spin coupling, described by $\boldsymbol{J}_{KL}$, between nuclei K and L, can be detected also in isotropic fluids. In it the magnetic moment of the nucleus K polarizes the magnetic moments of the electrons surrounding it and the magnetic fields generated by these electrons affect the experienced magnetic field of the nucleus L.

There are also cases, in which additional effects must be included to the nuclear spin Hamiltonian [31]. This needs to be done for instance when paramagnetic systems are studied or when the nuclei possess a nuclear spin $I_K > 1/2$ and therefore possess an electric quadrupole moment, which interacts with the gradient of the electric field at the site of the nucleus.

2.1.2. NMR shielding

NMR shielding is caused by an induced magnetic field that is usually opposite to the external magnetic field, thus lowering the total magnetic field that the nucleus experiences [26]. The induced magnetic field arises from the movement of the electrons around the nucleus. In experimental NMR this is observed as a relative shift in the frequency of the measured signal and it is described as the chemical shift δ (in ppm):

$$\delta = \frac{\nu - \nu_{\text{ref}}}{\nu_{\text{ref}}}. \tag{2.5}$$

In Equation (2.5), ν is the observed frequency and ν_{ref} is the frequency of a nucleus of interest in a reference compound such as TMS (tetramethylsilane) or in the case of this study, methane. By applying Equation (2.3) we can write ν as

$$\nu = \frac{\gamma}{2\pi}(1 - \sigma)B_0, \tag{2.6}$$

where σ is the so-called shielding constant and B_0 is now the external field. Therefore, the chemical shift can be written in the terms of shielding:

$$\delta = \frac{\sigma_{\text{ref}} - \sigma}{1 - \sigma_{\text{ref}}} \tag{2.7}$$

where σ_{ref} is the shielding constant of the reference compound. As the values of shielding constants are usually very small, we can write the chemical shift approximately as

$$\delta = \sigma_{\text{ref}} - \sigma. \tag{2.8}$$

2.2. Electronic structure calculations

If we want to study the chemical shift of graphane, we need to know it's electronic structure. For NMR calculations it is also crucial to have a realistic geometry of the investigated system. This can be achieved by careful evaluation of the electronic structure of the system.

The most common quantum-chemical method used today is DFT. It is based on electron density. It can be shown that the energy of the system can be written as a functional of electron density. This brings a big advantage for DFT compared to different *ab initio* methods, as DFT makes the calculations more cost effective. When using DFT, the energy of the system is also a functional of electron density. The theory of this section will be based on *Molecular Quantum Mechanics* by Atkins and Friedman [32].

2.2.1. Hamiltonian for electrons

The starting point for all electronic structure calculations lies in the time-independent Schrödinger equation that can be, in the simplest form, written as

$$\hat{H}\left|\Psi_i\right\rangle = E_i\left|\Psi_i\right\rangle, \tag{2.9}$$

where Ψ_i is the i:th state of the system, E_i is its energy and $\hat{H}$ is the Hamiltonian operator. The Born-Oppenheimer approximation states that we can consider the nuclei to be static in relation to the electrons. This is based on the approximation that the electrons respond immediately to the movements of the nuclei due to the big difference in mass. When the Born-Oppenheimer approximation is taken into account the Hamiltonian can be written as

$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i^{N_e}\nabla_i^2 - j_0\sum_i^{N_e}\sum_K^{N_n}\frac{Z_K}{r_{iK}} + \frac{j_0}{2}\sum_{i,j=1}^{N_e}\frac{1}{r_{ij}} = \hat{T} + \hat{V}_{ne} + \hat{V}_{ee} \tag{2.10}$$

where ∇_i^2 is the Laplace operator, $\hbar$ is the reduced Planck's constant, m_e is the mass of an electron and $j_0 = e^2/4\pi\epsilon_0$ (e is the elementary charge and ϵ_0 is the vacuum permittivity). The distances between electrons are marked as r_{ij} and correspondingly the distance between electron i and the nucleus K is marked as r_{iK}.

The first term of the operator, $\hat{T}$, is the operator for the kinetic energy of the electrons. The second term $\hat{V}_{Ne}$ is the operator for the potential energy between the electrons and the nuclei and the third term is the operator for the potential energy between the electrons. It is impossible to achieve an exact wavefunction in a complex system with many electrons. Therefore, an approximate method, such as DFT, is required.

2.2.2. Hohenberg-Kohn theorems

In 1964 P. Hohenberg and W. Kohn derived two theorems [33] that create the basis for DFT.

Theorem 1 *The ground-state energy E_0 and all the other ground state properties can be determined uniquely by the ground state electron density $\rho_0(\boldsymbol{r})$.*

Electron density of a system is defined as

$$\rho(\boldsymbol{r}) = \sum_{i=1}^{N_e}\left|\phi_i^{\mathrm{KS}}(\boldsymbol{r})\right|^2, \tag{2.11}$$

where $\phi_i(\boldsymbol{r})$ is the spin-orbital for electron i. The first theorem shows [32] that the ground state energy can be written as a functional of electron density

$$E[\rho] = \underbrace{T[\rho] + V_{\mathrm{ee}}[\rho]}_{=E_{\mathrm{HK}}[\rho]} + \int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r}, \tag{2.12}$$

where the first term is the kinetic energy for the electrons and the second term is the potential energy of the electrons. The sum of these two terms is called the Hohenberg-Kohn energy $E_{\mathrm{HK}}[\rho]$. The third term describes the interaction between the electrons and the nuclei where $v(\boldsymbol{r})$ is a so-called external potential, which affects the electrons by the nuclei. Because it is possible to show [32] that electron density solely defines the external potential, and naturally also the same applies for the ground state electron density, the properties of the investigated system can be determined by the electron density.

Theorem 2 *The energy E, defined by a trial electron density $\rho'(\boldsymbol{r})$, is an upper limit to the ground state energy E_0.*

The second theorem resembles the variational theorem. In this case we can write that

$$\langle \psi' | \, H \, | \psi' \rangle = E[\rho'] \geq E_0, \tag{2.13}$$

where the wavefunction ψ' is defined by trial electron density ρ'.

2.2.3. Kohn-Sham equations

A year later from the publication of the Hohenberg-Kohn theorems, Kohn and Sham created a method [29], that utilizes the theorems in a self-consistent manner, which can be used approximately to solve the electron density of a desired system.

Let us consider a reference system with N electrons similarly to a system of interest, but the electrons do not interact with each other. For this reference system we can write the Hamiltonian operator in the form

$$h_{\mathrm{ref}} = \sum_{i=1}^{N_e} h_i^{\mathrm{KS}}, \tag{2.14}$$

where h_i^{KS} is the so-called Kohn-Sham (KS) Hamiltonian for electron i. The KS Hamiltonian can be written as

$$h_i^{\mathrm{KS}} = -\frac{\hbar^2}{2m_e}\nabla_i^2 + v_{\mathrm{ref}}(\boldsymbol{r}_i). \tag{2.15}$$

The first term of the operator describes the kinetic energy of an electron in the non-interacting reference system. The second term is the potential energy that affects the electron. Eigenfunctions of the one-electron Hamiltonian operator are called KS-orbitals ψ_m^{KS} and they fulfill the following eigenvalue equation

$$h_i^{\mathrm{KS}}\phi_i^{\mathrm{KS}} = \varepsilon_i^{\mathrm{KS}}\phi_i^{\mathrm{KS}}, \tag{2.16}$$

where the eigenvalue $\varepsilon_i^{\mathrm{KS}}$ is the KS-orbital energy. The wavefunction Ψ_{ref} of the whole

reference system can be described by a Slater determinant.

$$\Psi_{\text{ref}}(1,2,\ldots,N_e) = \frac{1}{\sqrt{N_e!}} \begin{vmatrix} \phi_a(1) & \phi_b(1) & \ldots & \phi_z(1) \\ \phi_a(2) & \phi_b(2) & \ldots & \phi_z(2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_a(N_e) & \phi_b(N_e) & \ldots & \phi_z(N_e) \end{vmatrix}, \tag{2.17}$$

where ϕ^{KS} is a KS spin-orbital and N_e is the number of electrons. KS spin-orbitals also include the spin state of the electron.

The energy of the system can be solved using the first Hohenberg-Kohn theorem and Equation (2.12). The usefulness of the reference systems kicks in here, when we use it to determine the kinetic energy of the electrons in the real system. The kinetic energy of the reference electrons $T_{\text{ref}}[\rho]$ is smaller than the kinetic energy of the real electrons $T[\rho]$ but it can still be used. Only a small part of the energy will be left unknown. In a similar matter the classical Coulomb potential $J[\rho]$ between the electrons is only a part of the real potential energy between the electrons. By using the reference system, we can accurately determine this part. Now we can write the Equation (2.12) in the following form:

$$E[\rho] = (T[\rho] - T_{\text{ref}}[\rho]) + (V_{\text{ee}}[\rho] - J[\rho]) + \int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r} + T_{\text{ref}}[\rho] + J[\rho] \tag{2.18}$$

$$= E_{\text{XC}}[\rho] + \int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r} + T_{\text{ref}}[\rho] + J[\rho], \tag{2.19}$$

where $E_{\text{XC}}[\rho]$ is called the exchange-correlation functional. It can also be written as a sum of the exchange and correlation functionals:

$$E_{\text{XC}}[\rho] = E_{\text{X}}[\rho] + E_{\text{C}}[\rho]. \tag{2.20}$$

These two terms represent the exchange and correlation energies. The exchange energy arises from the Pauli exclusion principle, which states that two fermions (*e.g.*, electrons) cannot occupy the same quantum state [34]. The exchange-correlation functional is the only unknown part of the KS-DFT. In other words, all unknown parts of the energy of the system are summed up in one term [32].

By using the second Hohenberg-Kohn theorem it is possible to show [32] that solving the electron density for the realistic system is actually the same as solving it for the reference electrons in a so called effective potential $v_{\text{eff}}(\boldsymbol{r})$ which can be written as

$$v_{\text{eff}}(\boldsymbol{r}) = v(\boldsymbol{r}) + v_{\text{XC}}(\boldsymbol{r}) + j_0 \int \frac{\rho(\boldsymbol{r'})}{|\boldsymbol{r'} - \boldsymbol{r}|} d\boldsymbol{r'}, \tag{2.21}$$

where $v(\boldsymbol{r})$ is the potential between the nuclei and electrons, $v_{\text{XC}}(\boldsymbol{r})$ is the exchange-correlation potential and the last term is the classical Coulomb potential between the electrons. By replacing the $v_{\text{ref}}(\boldsymbol{r_i})$ with $v_{\text{eff}}(\boldsymbol{r_i})$ in Equation (2.15) we can write the

so-called Kohn-Sham equation as [32]

$$\left[-\frac{\hbar^2}{2m_e}\nabla_1^2 + v_{\text{eff}}(\boldsymbol{r_i})\right]\psi_m^{\text{KS}}(\boldsymbol{r}_i) = \varepsilon_m^{\text{KS}}\psi_m^{\text{KS}}(\boldsymbol{r}_i). \tag{2.22}$$

From this equation we can solve the KS-orbital of the system.

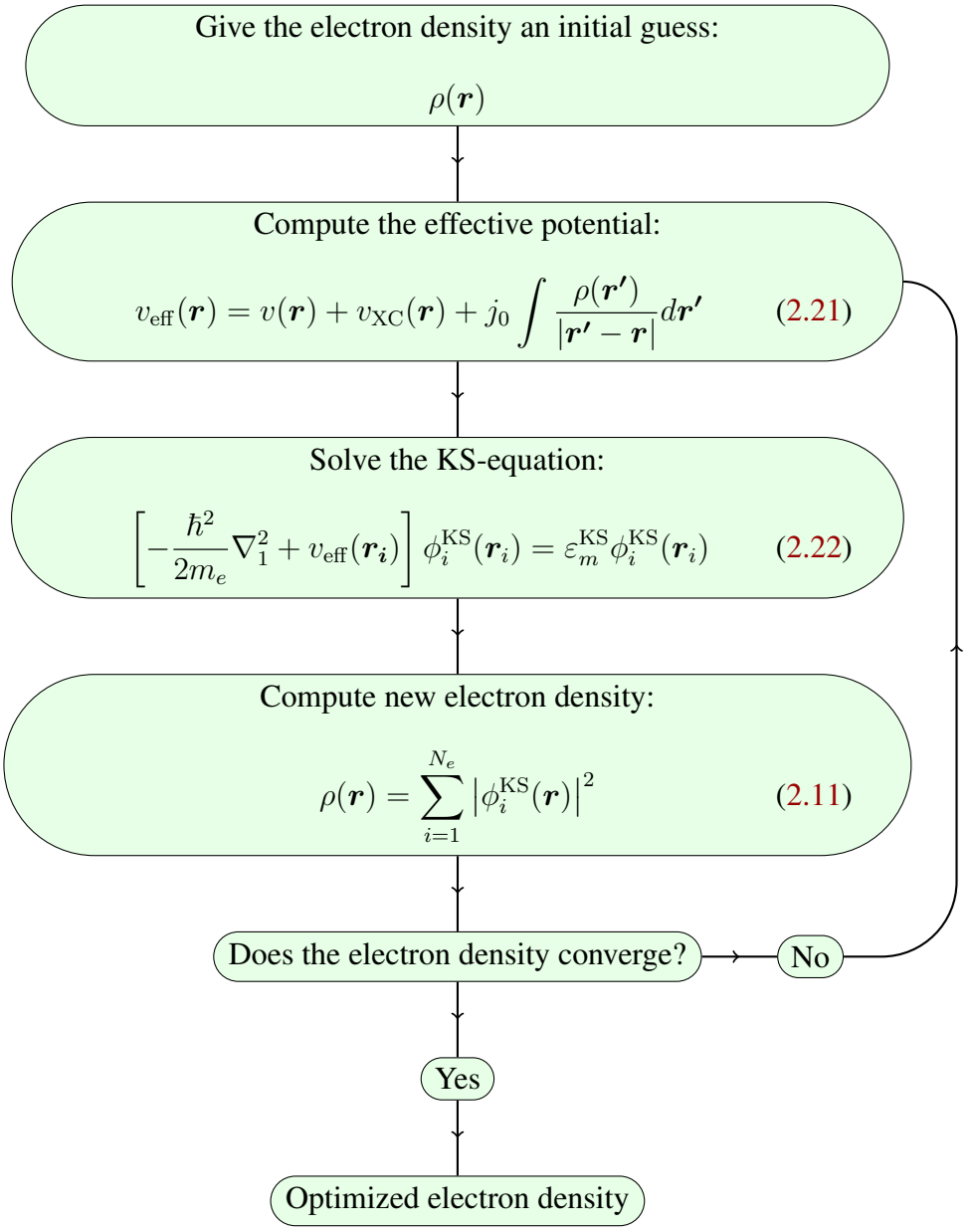

Figure 2.2: A flow chart describing the self-consistent way to solve the KS-equation in DFT.

In the KS-DFT the electron density is solved in a self-consistent manner. The whole procedure is showed in Figure 2.2. The first step of it is to give the electron density an initial guess. This is usually based on a superposition of the electron densities of individual

atoms. The next step is to solve the effective potential $v_{\text{eff}}(\boldsymbol{r})$ using Equation (2.21). With the initial electron density and the effective potential, we can solve the Equation (2.22). From the wavefunction we can form a new electron density of the system. The new electron density is mixed with the old density to achieve convergence. There are different methods for this and one of them is a simple linear mixing where the new starting density is formed as a sum of the old and new density with different mixing coefficients. This computational cycle is repeated so that the desired convergence is achieved [32].

As stated above, the only unknown term of the effective potential is the exchange-correlation potential which by definition can be derived from the exchange-correlation energy functional. The simplest approximations of this functional are the local density approximation (LDA) and the local spin density approximation (LSDA). Both rely on the approximation that the electronic system can be thought as homogeneous electron gas. The difference between these two types of functionals is that LSDA considers the electrons spins in an open-shell calculation. LDA and LSDA work fine with simple metals, such as sodium, but if the system is for example a single electron, where the electron density goes to zero as the distance from the nucleus increases, it doesn't work [35].

A more elaborate group of functionals are the generalized gradient approximations (GGAs). As their name states the functional also takes into account the gradient of the electron density. In most cases for molecules and also for solid state systems GGAs are far better than LDA or LSDA. In addition of LDA, LSDA and GGAs there are also so called hybrid functionals which are combination of a exact exchange functional from Hartree-Fock method and an approximate correlation functional [35].

Geometry optimization

Geometry optimization (energy minimization) is based on finding local minima of the potential energy surface (PES) of the investigated system [34]. This can be done by computing the forces acting on atoms.

$$\boldsymbol{F} = -\nabla E \tag{2.23}$$

If the forces are stronger than desired threshold values, the atoms of the system are moved to a different position closer to the predicted minimum and the forces are calculated again. This is repeated until the threshold value is achieved.

Zero values of forces in Equation (2.23) can, in addition to local minima, occur at local maxima or other saddle points [34]. Therefore it is reasonable to investigate also the sign of the second derivative $\boldsymbol{H_{ij}} = -\partial^2 E/\partial r_i \partial r_j$ to distinguish the type of the saddle point. The second derivative is called the Hessian matrix as it a square matrix of second-order

partial derivatives. In a general form for $f(\boldsymbol{x})$ it can be written as

$$\boldsymbol{H} = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1 \partial x_n} \\ \dfrac{\partial^2 f}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f}{\partial x_n \partial x_1} & \dfrac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}. \tag{2.24}$$

An example of a method used to solve the Hessian matrix in Equation (2.24) is the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm [36], which is used by Quantum ESPRESSO (QE) [37]. With the optimized geometry and the electron density, the NMR shielding can be determined by the GIPAW method [28], which is described in Subsection 2.3.2.

2.2.4. DFT for periodic systems

In a solid state system there can be practically an infinite number of electrons moving in an effective potential. A direct consequence of this is an infinite number of KS-orbitals. This problem can be solved by utilizing the periodic behavior of crystalline solid state matter.

In a crystalline lattice the atoms of the system are arranged in a periodic and ordered manner. A unit of this lattice is called an unit cell. The geometry of the whole system can be built by repeatedly moving the unit cell to the points of the Bravais lattice which are located at

$$\boldsymbol{T} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3, \tag{2.25}$$

where n_i are integers and $\boldsymbol{a}_i$ are so called lattice vectors which span the unit cell. The Fourier transform of this Bravais lattice can be written as

$$\boldsymbol{G} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2 + m_3\boldsymbol{b}_3. \tag{2.26}$$

Here the vectors $\boldsymbol{b}_i$ span the Fourier-transformed space that is called the reciprocal space. The unit cell in reciprocal space is called the first Brillouin zone. $\boldsymbol{G}$ is called the reciprocal lattice vector [35].

In practice, a set of basis functions are used to describe the wavefunction. There are several different variations for these. For molecules a popular choice are Gaussian-type orbitals (GTO) or Slater-type orbitals (STO). For periodic systems a natural choice of a basis function is the plane wave due to Bloch's theorem [38]. The theorem states that any one-electron wavefunction can be described with a plane wave in a periodic potential.

This wavefunction can then be written in reciprocal space as

$$\psi_{i,\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}} \sum_m c_{i,m}(\boldsymbol{k}) e^{i(\boldsymbol{k}+\boldsymbol{G_m})\cdot\boldsymbol{r}}, \tag{2.27}$$

where Ω is the volume of the unit cell, $\boldsymbol{k}$ is a wave vector that describes the momentum of the electrons in the Brillouin zone, i labels the band of eigenvalues and $c_{i,m}$ are the coefficients for the KS-orbitals [35].

The KS-equation for a periodic system using plane waves as a basis, is written as

$$\sum_{m'} \left[\frac{\hbar^2}{2m_e} |\boldsymbol{k} + \boldsymbol{G}_m|^2 \delta_{m,m'} + V_{\text{eff}}(\boldsymbol{G}_m - \boldsymbol{G}_{m'}) \right] c_{i,m'} = \epsilon_i(\boldsymbol{k}) c_{i,m}(\boldsymbol{k}), \tag{2.28}$$

where $V_{\text{eff}}(\boldsymbol{G}_m - \boldsymbol{G}_{m'})$ is the Fourier-transformed effective potential. The first term on the left hand side describes the kinetic energy of the electrons [35].

If not limited, the size of the kinetic energy term is infinite. For practical calculations there has to be some upper limit to the term:

$$E_{\text{cutoff}} \geq \frac{\hbar^2}{2m_e} |\boldsymbol{k} + \boldsymbol{G}_m|^2. \tag{2.29}$$

In calculations the kinetic cutoff energy E_{cutoff} determines the size of the used basis set. It has to have high enough value so that the results are accurate. However, it should also be reasonable as the calculation will get heavier as its value gets higher. It is therefore desirable to do convergence test to find out the optimal value for the kinetic energy cutoff [4].

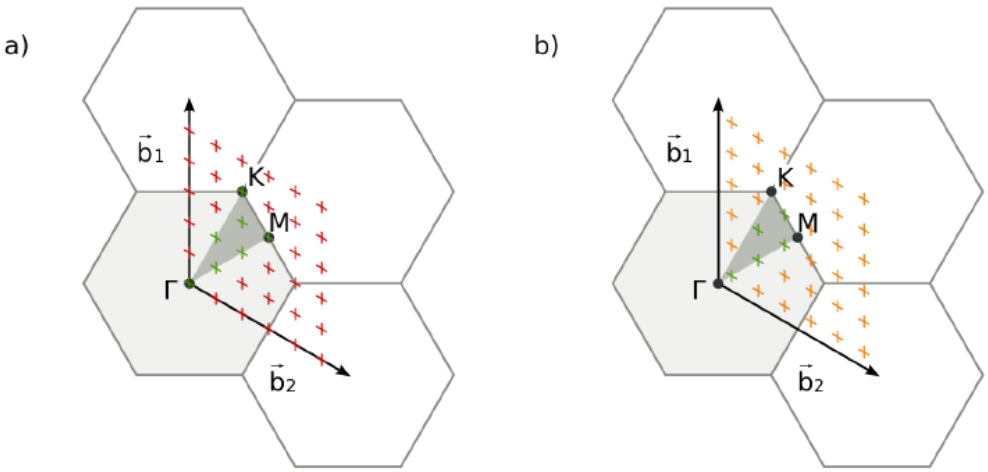

Figure 2.3: Example of the k-point sampling of the Brillouin zone in a hexagonal lattice. Points Γ, K and M are so-called points of high symmetry. In subfigure a), the sampling is a $6 \times 6 \times 1$ (in case of a 2D system) k-point grid which is centered at Γ and in b) it is the same but not centered at Γ [40].

According to Equation (2.27) there are also an infinite number of k-points set by the wave vectors $\boldsymbol{k}$. Similarly to the cutoff energy, the number of k-points has to be limited for practical calculations. The sufficient number of k-points is chosen so that the energy and the electronic density become accurate enough. This is also done by convergence tests.

By using a small number of k-points it must be made sure that the k-points sample the Brillouin zone accurate enough. Monkhorst and Pack [39] have developed a method for sampling the k-points in the Brillouin zone by using an uniform distribution of k-points along the basis vectors of the reciprocal unit cell. An example of the Monkhorst-Pack method is displayed in Figure 2.3.

2.2.5. PAW and pseudopotentials

Most of the properties of molecules and solid state materials are determined by the valence electrons. In the solid state, the valence electrons are often thought to be very loosely bound to the nuclei and therefore treated as they were delocalized in the lattice. On the other hand, core electrons are very tightly bound with the nuclei and they do not significantly affect the properties of the matter. However, they are problematic in practical calculations due to the fact that, near the nuclei, the potential energies get higher and more plane waves are needed to describe the wavefunction of the electronic system. This makes the practical calculation eventually impossible [4].

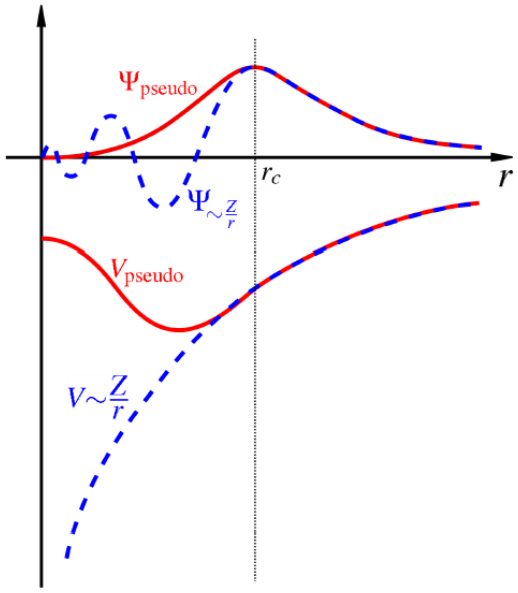

Figure 2.4: Pseudopotential V_{pseudo} simplifies the wavefunction Ψ in the core region ($r < r_c$). [43]

Pseudopotentials mimic the real potentials of the system in the valence region but are much weaker in the core region as seen in the sketch in Figure 2.4. Using them the wave function of the system is close to the real one in the valence region but it is has

significantly less nodes in the core region and therefore it is possible to reduce the size of the used basis set. Common types of pseudopotentials are so called norm-conserving (NC) pseudopotentials [41] and ultrasoft (US) pseudopotentials [42].

The projector-augmented wave method (PAW) [44] enhances the accuracy of the use of pseudopotentials for two main reasons. Firstly, the distance from the nucleus in which the potential is altered can be smaller when using PAW method. Secondly, it recreates the oscillations of the wavefunction in the core region. This is very crucial for calculating the NMR shielding, which is mainly caused by the core electrons [4, 45].

2.3. Calculation of the NMR shielding tensor

The NMR shielding tensor in Equation (2.4) can be defined by the induced magnetic field $\boldsymbol{B}_{\mathrm{ind}}(\boldsymbol{r'})$ and the external magnetic field $\boldsymbol{B}_0$ [46]:

$$\boldsymbol{B}_{\mathrm{ind}}(\boldsymbol{r'}) = -\boldsymbol{\sigma}(\boldsymbol{r'}) \cdot \boldsymbol{B}_0. \tag{2.30}$$

The induced magnetic field can be solved from the Biot-Savart law:

$$\boldsymbol{B}_{\mathrm{ind}}(\boldsymbol{r'}) = -\frac{1}{c^2} \int \frac{\boldsymbol{j}(\boldsymbol{r}) \times (\boldsymbol{r} - \boldsymbol{r'})}{|\boldsymbol{r} - \boldsymbol{r'}|^3} d\boldsymbol{r}. \tag{2.31}$$

where $\boldsymbol{j}(\boldsymbol{r})$ is the current density that can be solved using a converged electron density. The problem at hand is therefore to determine the current density. This can be done by solving the electron density of the system using DFT but we also have to take into account the effects of the external magnetic field.

2.3.1. Cluster approach

In the cluster approach we can use the quantum chemical approach, which is an approach designed for molecules, for solid state materials. The basic idea is that we just create a finite cluster of the investigated periodic system and treat it like a molecule. By that we can use sophisticated quantum chemical methods to determine for example the NMR shielding for the nuclei in the middle of the cluster. By increasing the size of the cluster, its edge will not affect the center that much and therefore we can mimic the periodic structure of the real graphane. The convergence of the shielding in the middle of the cluster should be studied, when using this sort of a approach.

However, the method has its own problems [47]. The boundaries of the cluster affect its NMR properties all around the cluster. There are also problems with for instance with the HOMO-LUMO gaps. Despite the problems it has been used to investigate NMR properties of graphane systems and with big enough cluster sizes the shielding does converge in the middle of the cluster close to the value that can be achieved using methods created specifically for periodic systems [27, 48, 49]. This is possible due to the local nature of hyperfine interactions [48, 50].

As noted earlier, for all practical calculations we need to use some set of functions as a basis to describe the orbitals. A simple method for this when working with molecules is the LCAO (Linear Combination of Atomic Orbitals). It can be used to build complicated molecular orbitals from simple atomic orbitals as a linear combination [32]. Mathematically this can be written in a simple form:

$$\phi_i = \sum_r c_{r,i}\chi_r, \tag{2.32}$$

where ϕ_r is a atomic orbital and c_r is a corresponding multiplication coefficient. The most used basis set for these atomic orbitals are Gaussian-type orbitals (GTOs) [32].

The orbitals generated using LCAO and for example GTOs are not exact because it is impossible to use an infinite sized basis set in a practical calculation. This gives rise to a so-called gauge origin problem [51]. It arises from the vector potential of the external magnetic field [45]

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{B}_0 \times (\boldsymbol{r} - \boldsymbol{r}_0). \tag{2.33}$$

For exact wavefunctions it is possible to show that the current density is not dependent of choice of gauge origin $\boldsymbol{r}_0$ [46]. However, when the wavefunctions are built from a finite set of basis functions, the choice of gauge origin affects the calculated NMR shielding constant.

For the purpose of demonstration let us consider a methane molecule and try to determine the shielding constant for one of its ^{1}H nuclei using a fixed gauge origin and different basis sets to describe the orbitals. The basis sets used here are pcS-n basis sets [52]. When n gets higher, the basis set size increases and it produces more accurate results. From Table 2.1 we see that the location of the gauge origin affects greatly the shielding when we use a small basis sets. However, when we increase the size of the basis set we notice that the results start to converge. The problem with bigger basis sets is that the calculation itself becomes slow and costly.

Table 2.1: Values of ^{1}H NMR shielding constants for methane using DFT. Calculations were performed with Dalton2016 [55] using different basis sets with fixed gauge origins and with the GIAO method. The used exchange-correlation functional is KT3 [56].

Basis set	Common gauge origin			GIAO
	H (same)	H (different)	C	
pcS-0	65.53	16.54	28.79	32.78
pcS-1	42.65	27.77	31.49	31.64
pcS-2	36.20	29.98	31.54	31.80
pcS-3	31.86	31.77	31.79	31.79

GIAO (Gauge-Including Atomic Orbital) [53, 54] is a commonly used method that takes care of the gauge origin problem. The basis set functions are expanded with atomic orbitals that include the gauge origin [51]. Because of this, the gauge dependence of NMR

shielding disappears. When using the GIAO method for the methane molecule, we notice from Table 2.1 that the value of the shielding constant converges much faster than it does when the gauge origin is fixed to a common location in the molecule.

2.3.2. Gauge-Including Projector Augmented Wave Method

In addition to quantum chemical NMR approaches, first-principles methods for periodic materials are also important in chemistry and materials science today [57]. GIPAW (Gauge-Including Projector Augmented Wave) method [28], based on a previous MPL (Mauri, Pfrommer and Louie) method [58, 59], can be used for the computational study of NMR shielding, spin-spin coupling and quadrupolar interaction in solid state materials including graphane systems.

In this method the NMR shielding tensor can be written as a sum of four terms:

$$\boldsymbol{\sigma} = \sigma_{\text{core}}\mathbf{1} + \boldsymbol{\sigma}_{\Delta d} + \boldsymbol{\sigma}_{\Delta p} + \boldsymbol{\sigma}_{\text{bare}}. \tag{2.34}$$

Above, σ_{core} is the contribution from the electrons in core region to the shielding. The three latter terms are correction terms to the first one. $\boldsymbol{\sigma}_{\Delta d}$ is the so-called diamagnetic term and in a similar manner $\boldsymbol{\sigma}_{\Delta p}$ is the paramagnetic term. These terms correct the shielding from the changes that the use of pseudopotentials generates in the core region. The last term $\boldsymbol{\sigma}_{\text{bare}}$ is the contribution of the pseudo valence region electrons to the shielding. The efficiency of the method was improved in 2007 by Yates *et al.* [60] as the usage of ultrasoft pseudopotentials was made possible. This allowed a broader approximation of the core region with a higher accuracy. Also, the used cutoff energy could now be smaller.

A more detailed theoretical look on the method is shown for example in a review work done by Bonhomme *et al.* [57]. The main idea is to solve the electronic current density which is needed to compute the induced magnetic field in Equation (2.31). In an experimental setup, the magnetic fields are relatively small and so is the current density. Therefore, it is appropriate to apply perturbation theory. Also, the periodic behavior of a solid state material can be utilized and only a unit cell needs to be considered.

3. Computational details

The aim of this study is to product computational NMR chemical shifts for pure and graphene defected graphane-systems. Before the actual calculation extensive tests for computational parameters must be made to ensure accurate results with a moderate computational cost. After a careful selection of parameters, the geometries of the studied systems are optimized. Only then the NMR chemical shifts can be determined. In this chapter the computational process of this study will be explained in detail. All of the calculations were performed using Quantum ESPRESSO (QE) version 5.3.0 [61, 62] and all the figures of the investigated systems in this thesis were created from the optimized geometries using Avogadro [63] and VMD [64, 65].

3.1. Convergence tests

As noted earlier, it is crucial to optimize geometry accurately when computing NMR chemical shifts. To get accurate geometries for the investigated systems, computational parameters, such as cutoff energies and k-point sampling, must be chosen so that they do not affect the results. On the other hand, it is not desirable to use overly tight values for these parameters and increase the computational cost. Therefore, cutoff energies and the sampling of k-points were first tested with convergence tests for both the geometry optimizations and the NMR calculations. All of the pseudopotentials used in the testing are listed with their original filenames in Table 3.1. Pseudopotential files in this work were downloaded from the home page of QE and from Davide Ceresoli's homepage [66, 67].

Table 3.1: Exact filenames for different pseudopotentials used in this study. PP stands for pseudopotential type and XC for the exchange-correlation functional.

PP	XC	Atom	Filename
US	PBE [68]	C	`C.pbe-rrkjus-gipaw-dc.UPF`
		H	`H.pbe-rrkjus-gipaw-dc.UPF`
US	PBEsol [69]	C	`C.pbesol-n-rrkjus_psl.0.1.UPF`
		H	`H.pbesol-rrkjus_psl.0.1.UPF`
PAW	PBE	C	`C.pbe-n-kjpaw_psl.0.1.UPF`
		H	`H.pbe-kjpaw_psl.0.1.UPF`
PAW	PBEsol	C	`C.pbesol-n-kjpaw_psl.0.1.UPF`
		H	`H.pbesol-kjpaw_psl.0.1.UPF`

Reference values

In order to express results in the form of chemical shifts $\delta\,(\mathrm{ppm})$, reference values for absolute shieldings are needed. Methane (CH_4) is a simple hydrocarbon molecule that can be and has been used [27] as a reference for graphane systems. For the NMR calculations of methane, it is crucial to use big enough unit cell so that the methane molecules do not interact with each other notably. Hence the distances between molecules were set to be at least $20\,\text{Å}$. The geometry optimization and NMR calculations were performed using the same parameters that will be discussed in this chapter as for the pure graphane systems. The following results were obtained: $\sigma_\mathrm{C} = 187.06\,\mathrm{ppm}$ and $\sigma_\mathrm{H} = 30.85\,\mathrm{ppm}$. These reference values are used in Equation (2.8) when calculating the NMR chemical shift from the computed value of the NMR shielding constant.

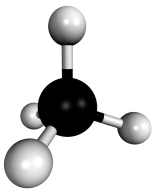

Figure 3.1: Methane (CH_4) was used as a reference molecule.

Vähäkangas *et al.* [27] computed the same values to be $\sigma_\mathrm{C} = 186.49\,\mathrm{ppm}$ and $\sigma_\mathrm{H} = 31.07\,\mathrm{ppm}$ using a periodic method. With a quantum chemical method the values were $\sigma_\mathrm{C} = 187.17\,\mathrm{ppm}$ and $\sigma_\mathrm{H} = 31.11\,\mathrm{ppm}$. The values differ from the ones calculated here, but for the 1-layer pure graphane systems a bigger difference between the results is seen. The difference is caused most likely by the use of different pseudopotentials, which his is discussed in detail in the Results and discussion chapter. For comparing the chemical shifts from this study to experimental spectra, which usually are in reference to TMS (tetramethylsilane), the difference between methane (an average solution state shift) with respect to TMS has been reported to be $\delta(\mathrm{TMS}) - \delta(\mathrm{CH_4}) = -4.6\,\mathrm{ppm}$ [70].

For the chair conformation of graphane, Vähäkangas *et al.* [27] computed the values of shielding constants to be $\sigma_\mathrm{C} = 121.89\,\mathrm{ppm}$ and $\sigma_\mathrm{H} = 30.66\,\mathrm{ppm}$. Therefore the values of chemical shifts were $\delta_\mathrm{C} = 64.60\,\mathrm{ppm}$ and $\delta_\mathrm{H} = 0.41\,\mathrm{ppm}$. Using the cluster method they calculated the NMR shielding of graphene to be $\sigma_\mathrm{C} = 132.18\,\mathrm{ppm}$ and therefore the value of chemical shift was $\delta_\mathrm{C} = 54.99\,\mathrm{ppm}$. The size of the cluster was G5, *i.e.*, it had five concentric carbon rings. The geometry of the system was adapted from optimized periodic system.

3.1.1. Geometry optimization

Idea of the convergence tests in geometry optimization is to analyze the behavior of total energy as a function of the computational parameters. All of the convergence tests for optimizing geometry were calculated using a PAW-pseudopotential [71] and a PBEsol exchange-correlation functional [69]. No van der Waals correction for dispersion was used in the convergence tests.

The tests were performed using the 1-layer chair conformation. The unit cell for the calculations was built using optimized geometry from previous research done by He *et al.* [21]. Height of the unit cell (the perpendicular direction to the graphane plane) was set to 20 Å to minimize interactions between layers. In a similar study made by Vähäkangas *et al.* [27] the distance between layers was set to be 18 Å and He *et al.* [21] used 15 Å. Therefore, we can assume that the height of 20 Å is big enough and no testing for it is needed in this case.

Kinetic energy cutoff E_{cutoff} for wavefunctions was tested using a $8 \times 8 \times 1$ k-point sampling and cutoff energies $E_{\text{cutoff}} = 10\,\text{Ry}, 15\,\text{Ry}, \ldots, 50\,\text{Ry}$. The total energy of the chair system is plotted in Figure 3.2 as a function of the cutoff energy. The cutoff energy for the charge density was always eight times larger than the corresponding cutoff energy for the wavefunction. From the figure we can see that the cutoff energy has converged at the value $40\,\text{Ry}$.

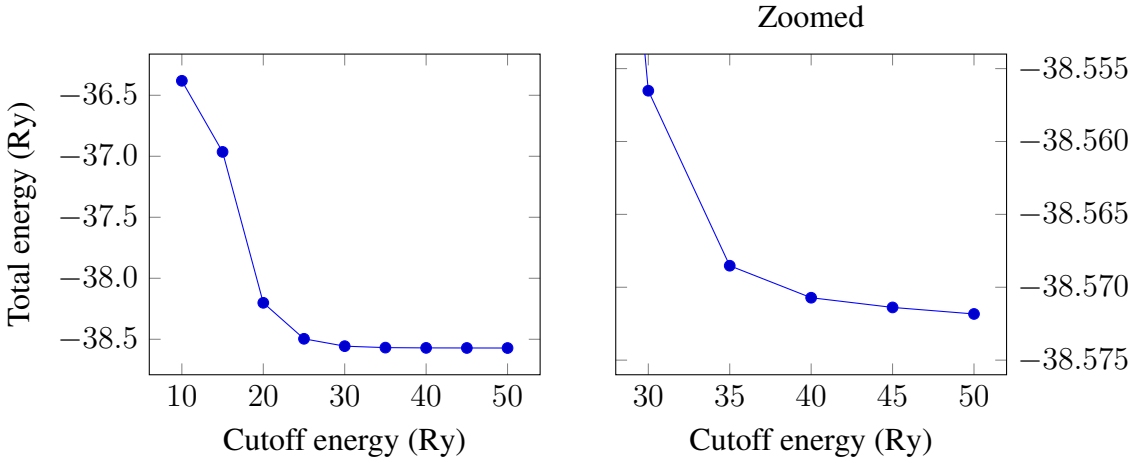

Figure 3.2: Total energy (Ry) as a function of the wavefunction cutoff energy (Ry).

Analogously, the convergence for the cutoff energy of the charge density was tested. The cutoff energy for the wavefunction was set to the converged value of $40\,\text{Ry}$. The k-point sampling was set to $6\times6\times1$. All values for total energy with different cutoffs were inside $0.0001\,\text{Ry}$ so the charge density cutoff doesn't seem to affect the results a great deal. It was chosen to be ten times higher ($400\,\text{Ry}$) than the wavefunction cutoff for the actual geometry optimization based on the input file description of QE [37].

A convergent k-point sampling was found using $30\,\text{Ry}$ as the cutoff energy of the wavefunction and $240\,\text{Ry}$ as the cutoff energy of the charge density. The sizes of used k-point samplings to calculate the total energy were $n\times n\times1$ where $n = 6, 8, \ldots, 18$. In this study the choice of convergent sampling was $6\times6\times1$ as the values of total energies with different k-point samplings were all between $-38.5550\,\text{Ry}$ and $-38.5555\,\text{Ry}$. Therefore, the smallest sampling is big enough as differences are small compared to the ones in Figure 3.2.

For all other conformations the same convergent cutoffs can be used. The same convergent *k*-point sampling cannot be used because of the different unit cell sizes. However, the same *k*-point density is convergent in the other conformations as well. We therefore only have to use a *k*-point sampling which has the same or lower distance between *k*-points in reciprocal space that of chair's which was in this case $0.08\,\text{Å}^{-1}$ in the direction of the graphane plane and $0.07\,\text{Å}^{-1}$ in the direction of the normal to the plane. The samplings for all conformations are listed in Table 3.2.

Table 3.2: *k*-point samplings for different graphane conformations for the geometry optimizations and for the NMR calculations. Underlined *k*-points indicate the direction of the normal to the graphane plane.

Conformation	*k*-point grid	
	Geometry optimization	NMR calculation
chair	$6 \times 6 \times \underline{1}$	$12 \times 12 \times \underline{1}$
boat-1	$5 \times 3 \times \underline{1}$	$10 \times 6 \times \underline{1}$
boat-2	$\underline{1} \times 3 \times 3$	$\underline{1} \times 6 \times 6$
stirrup	$5 \times \underline{1} \times 4$	$10 \times \underline{1} \times 7$
twistboat	$1 \times \underline{1} \times 5$	$6 \times \underline{1} \times 6$
tricycle	$\underline{1} \times 2 \times 5$	$\underline{1} \times 4 \times 11$

Different pseudopotentials and exchange-correlation functionals, which in QE are included in the pseudopotential file, were also tested. The testing was done by optimizing chair conformation's geometry using different pseudopotential files. The differences between optimizations can be analyzed by comparing carbon-carbon and carbon-hydrogen bond lengths. Used exchange-correlation functionals, pseudopotential types and bond lengths are given in Table 3.3. Bond lengths from two other studies [21, 27] are also reported.

Table 3.3: Carbon-carbon $d_{cc}\,(\text{Å})$ and carbon-hydrogen $d_{ch}\,(\text{Å})$ distances for 1-layer chair system in different studies. FCT stands for force convergence threshold value, PP for pseudopotential type and XC for the exchange correlation functional.

	Cutoff (Ry)	*k*-points	FCT (eV/Å)	XC	PP	$d_{cc}\,(\text{Å})$	$d_{ch}\,(\text{Å})$
	40	$6 \times 6 \times 1$	$2.6 \cdot 10^{-3}$	PBE	US	1.534	1.110
				PBE	PAW	1.535	1.110
				PBEsol	US	1.525	1.115
				PBEsol	PAW	1.526	1.115
[27]	48	$12 \times 12 \times 1$	$5 \cdot 10^{-6}$	PBE	US	1.534	1.110
[21]	37	$12 \times 12 \times 1^a$	$1 \cdot 10^{-2}$	GGA [72]	PAW	1.537	1.110
[73]	44	$10 \times 10 \times 1$	$1 \cdot 10^{-2}$	PBE	US	1.534	-

[a] Reciprocal distance between *k*-points was $0.21\,\text{Å}^{-1}$.

An important parameter for the geometric optimization is a convergence threshold on forces (`forc_conv_thr`). It sets an upper limit for the forces affecting the atoms in the system. For the criteria to be filled, all components of the forces must be smaller than the given value. In this study the used value for all of the calculations was $2.6 \cdot 10^{-3}\,\mathrm{eV/Å}$. The threshold values of other studies are also listed in Table 3.3.

By using the PBE functional and US pseudopotential we achieve same results as in work done by Vähäkangas *et al.* The PBEsol functional gives slightly shorter carbon-carbon bond lengths but longer carbon-hydrogen bond lengths. The pseudopotential type doesn't seem to affect the bond lengths as much as the functionals do in this case. Because of the similar results, geometry optimization was done in this study with the PBE functional and US pseudopotential.

The used calculation mode for geometry optimization in QE was `vc-relax` where `vc` stands for variable cell. These calculations therefore also optimize the lattice parameters. In order to keep the $20\,\text{Å}$ vacuum between the layers a constraint was set so that the lattice parameters only change in the direction of the plane.

In QE there is also a converge threshold value (`conv_thr`) for the self-consistency [37]. It is an upper limit for a estimated energy error of the calculation. For all of the geometric optimizations in this study the threshold was $1 \cdot 10^{-8}\,\mathrm{Ry}$ and for the NMR calculations it was $1 \cdot 10^{-10}\,\mathrm{Ry}$.

3.1.2. NMR calculations

NMR shielding was calculated for all systems mentioned above. Calculations were performed with QE-GIPAW. Similarly to the geometry optimization, also for the NMR calculation convergence tests must be performed. Converging of the absolute shielding was analyzed as a function of the cutoff energies and *k*-point samplings with different pseudopotentials.

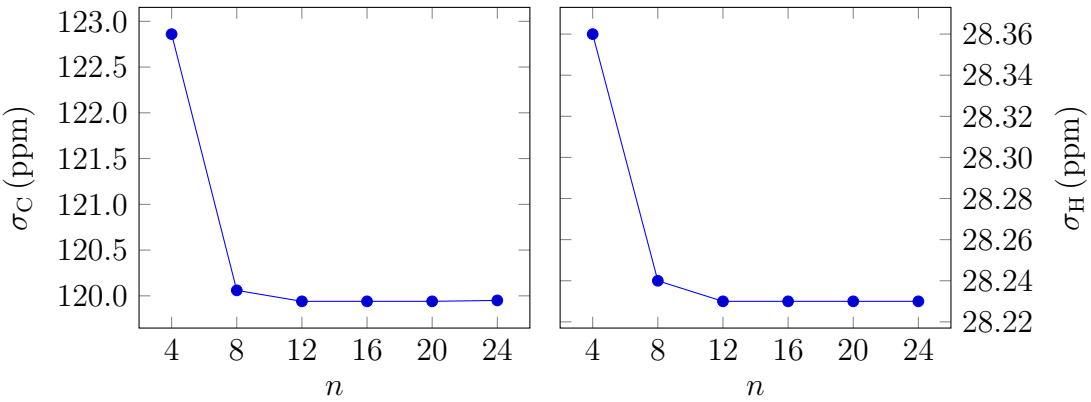

Figure 3.3: Absolute shielding for carbon $\sigma_C\,(\mathrm{ppm})$ and hydrogen $\sigma_H\,(\mathrm{ppm})$ as a function of $n \times n \times 1$ sized *k*-point sampling.

k-point sampling convergence was tested by calculating absolute shielding for the 1-layer chair system using a $40\,\mathrm{Ry}$ wavefunction cutoff, $400\,\mathrm{Ry}$ charge density cutoff, a

PBE exchange-correlation functional and a PAW potential. The results are displayed in figure 3.3 for both carbon and hydrogen. Convergence is achieved at a $12 \times 12 \times 1$-sampling. With higher sizes of samplings the value of absolute shielding for $^{13}\mathrm{C}$ changes at most $0.01\,\mathrm{ppm}$ and for $^{1}\mathrm{H}$ the values do not change at all. Hence for the actual NMR-calculations the upper limit for the *k*-point density is $0.04\,\text{Å}^{-1}$ in the direction of the plane and $0.07\,\text{Å}^{-1}$ in the direction of vacuum between the planes.

Similarly, the convergence of the absolute shielding was analyzed as a function of wavefunction cutoff energy. This was done both using a US pseudopotential and a PAW potential. In both cases a PBE exchange-correlation functional and a $15 \times 15 \times 1$ *k*-point grid was used. In Figure 3.4 and in Figure 3.5 the convergence can be seen in both cases around $70\,\mathrm{Ry}$, which was chosen to be the cutoff value for the actual NMR-calculations. With higher values of cutoff energy the absolute shielding can change for $^{13}\mathrm{C}$ at most by $0.02\,\mathrm{ppm}$ and, for $^{1}\mathrm{H}$, $0.07\,\mathrm{ppm}$.

The charge density cutoff was also tested using a US pseudopotential, PBE functional, $12 \times 12 \times 1$ *k*-point sampling and wavefunction cutoff of $70\,\mathrm{Ry}$. Again, it converges very quickly. Both for carbon and hydrogen the absolute shielding values are inside $0.04\,\mathrm{ppm}$ when the cutoff is higher than $200\,\mathrm{Ry}$. In the actual calculations, a value of $560\,\mathrm{Ry}$ was used.

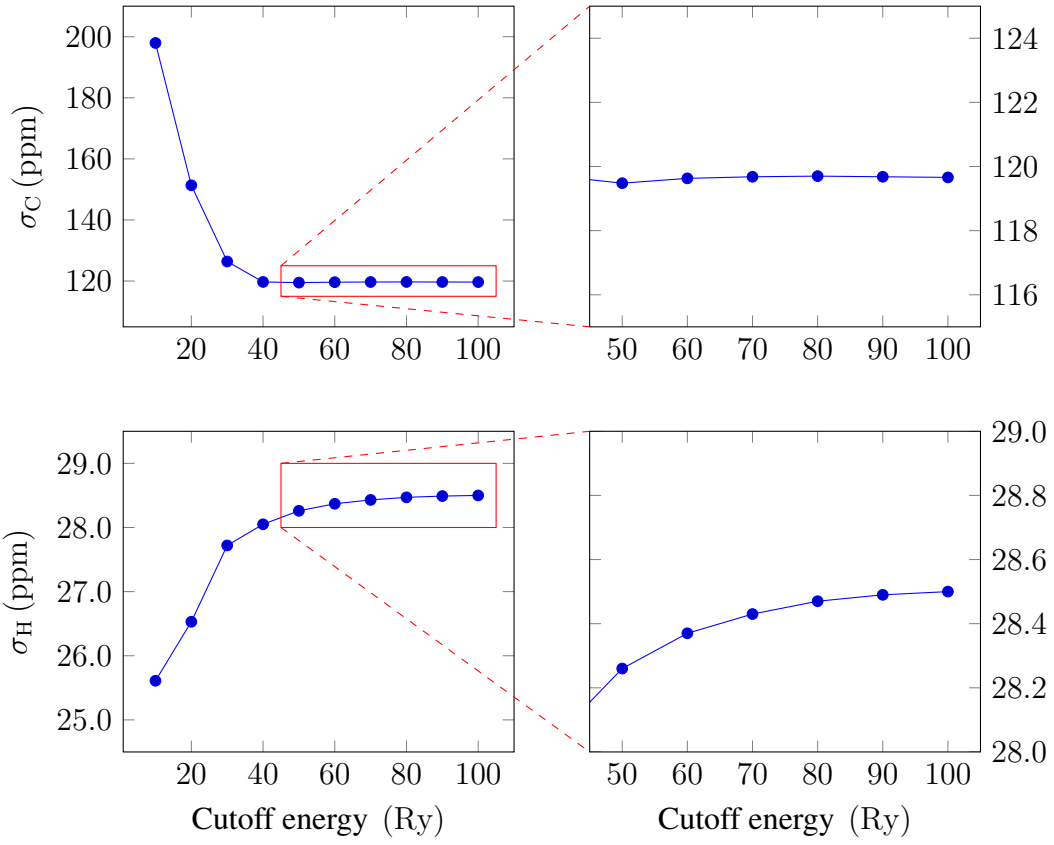

Figure 3.4: Absolute shielding for carbon $\sigma_{\mathrm{C}}\,(\mathrm{ppm})$ and hydrogen $\sigma_{\mathrm{H}}\,(\mathrm{ppm})$ as a function of wavefunction cutoff energy (Ry) using an US pseudopotential.

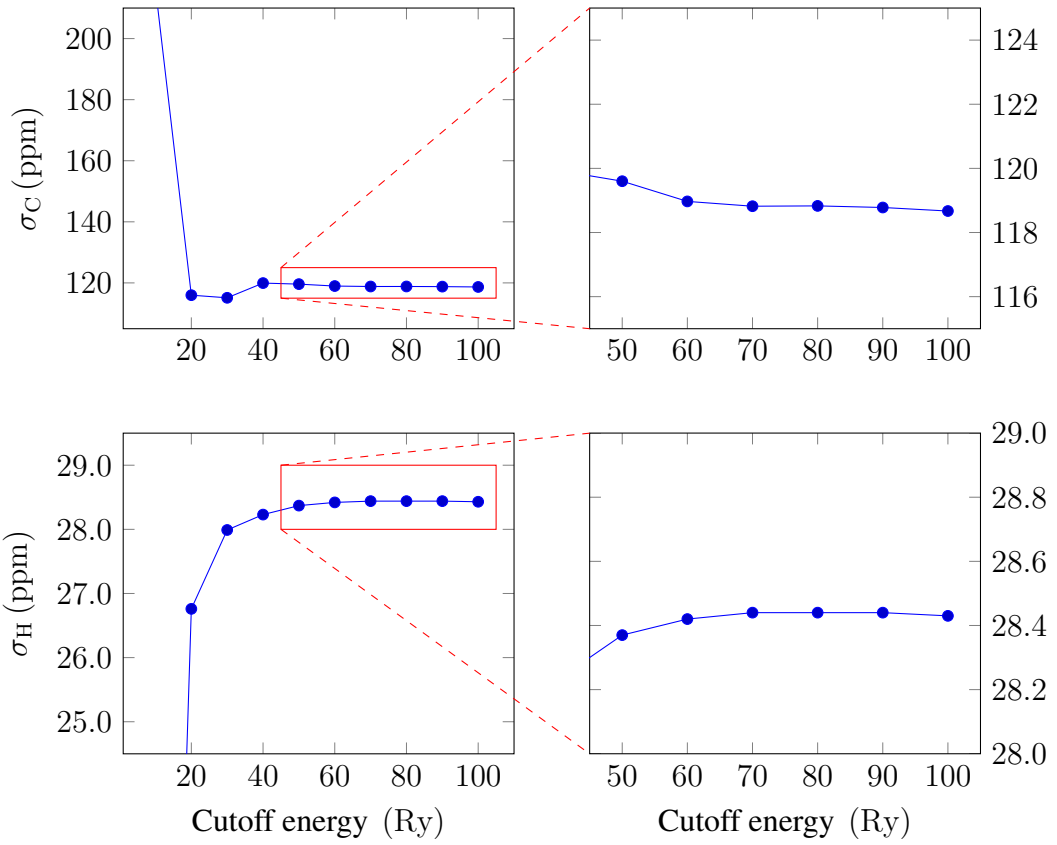

Figure 3.5: Absolute shielding for carbon σ_C (ppm) and hydrogen σ_H (ppm) as a function of wavefunction cutoff energy (Ry) using a PAW potential.

3.2. Pure graphanes

1-layer systems

1-layer models of all of the six conformations, chair, boat-1, boat-2, stirrup, twistboat and tricycle, were built from the optimized geometries of the study made by He *et al.* [21]. Also, the same naming convention was adapted for clarity. Cutoffs and *k*-point samplings (Table 3.2) were chosen according to convergence tests. For these actual geometry optimizations a van der Waals correction [74] was used. This affected the carbon-carbon bond lengths in the chair conformation compared to the testing values in Table 3.3. The optimized systems are displayed Figure 3.6 with the carbon-carbon and carbon-hydrogen bond lengths in Ångstroms.

NMR-calculations for the 1-layered systems were performed using the converged parameters (Table 3.2, Table 3.3). An ultrasoft pseudopotential with the PBE functional was used. Results of the calculations are displayed and discussed in the Results and discussion chapter.

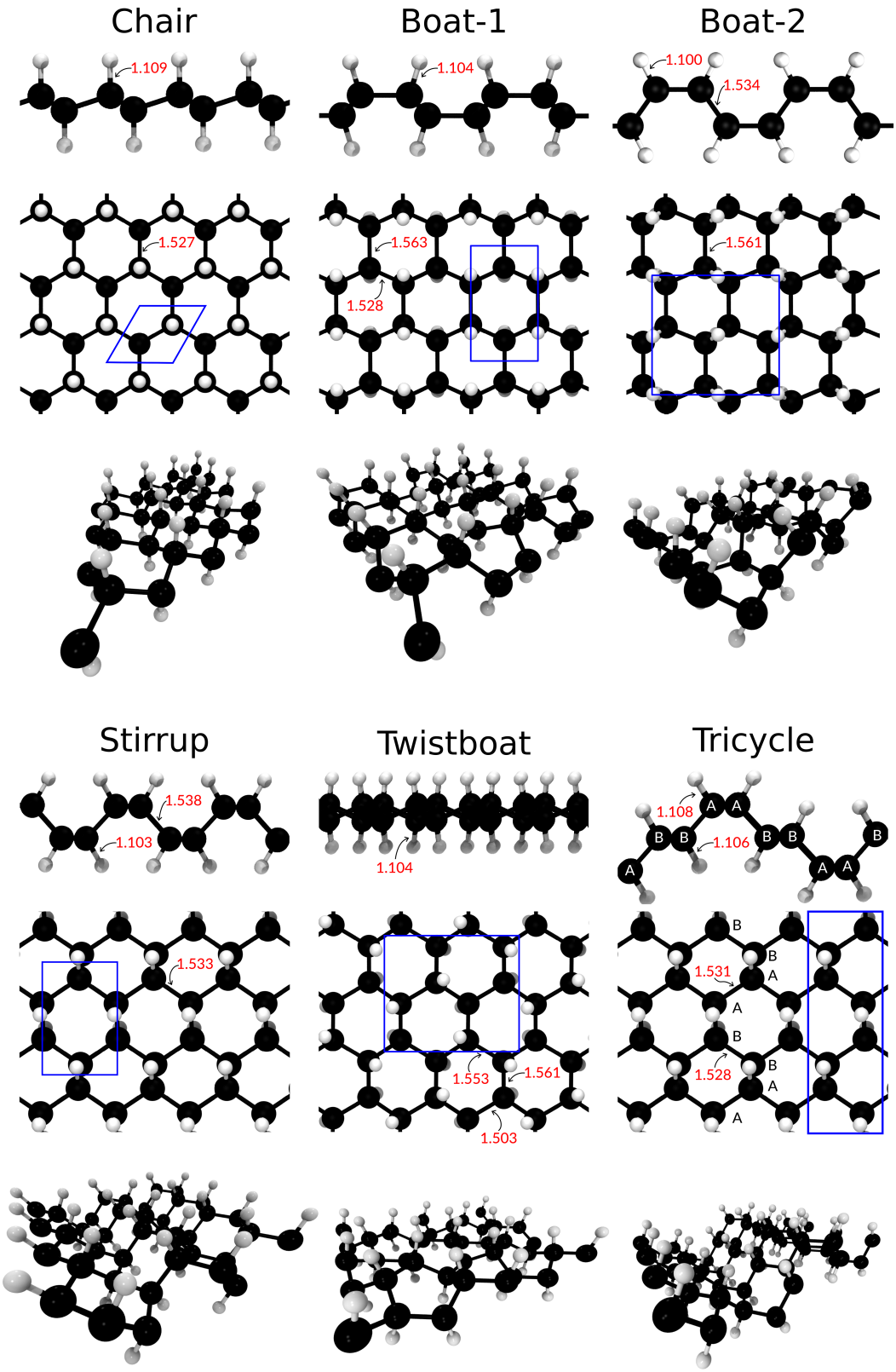

Figure 3.6: Side, up and perspective views of different 1-layer systems. Unit cell is displayed from above with the blue lines. Distinct carbon sites are indicated for the tricycle conformation using capital letters. Bond lengths are in Å.

Stacked systems

The starting geometries for all of the stacked systems were built using the optimized geometries from 1-layer systems. The 2-layered models were created by adding another set of unit cell atoms below the original atoms from 1-layer system. The starting distance between the layers was chosen to be around 6 Å. The size of the vacuum was also increased so that the distance between layers in different unit cells was again at least 20 Å.

Two styles of stacking were used: aa-stacking and ab-stacking. For the chair conformation both were created and for the others only the ab-stacking was used. The aa-stacked system was built so that the two layers were directly above each other. For the ab-stacked systems the other layer of atoms in the unit cell was shifted in the direction of the plane so that the atoms were no longer directly above another. No constraint for the optimization was set except the restriction to change the height of the unit cell. In the case of tricycle, the set ab-stacking did not hold and the optimization forced the system into the aa-stacked version.

In the same convention the 3-layered and bulk systems were created from the 2-layer models. For the chair conformation 3-layered systems with aaa- and aba-stackings were built by adding an extra layer of atoms into the unit cell. In a similar manner aba-stacked systems of other conformations were generated. Again, the tricycle conformation was changed to aaa-stacked system by the geometry optimization. The bulk systems were built by removing the vacuum between unit cells from the 2-layer systems. Also, the constraint on the unit cell height optimization was removed.

Geometry optimizations of stacked systems were performed using the same computational parameters as for the 1-layer systems. Pictures of the optimized systems can be seen in Figure A.1, Figure A.2 and Figure A.3. Also the NMR calculations were carried out using the same cutoffs but the *k*-point samplings differed a bit. For all stacked systems, except the 3-layered chair systems, the number of used *k*-points in the direction of the vacuum was two.

For the bulk chair-aa and chair-ab the effect of changing the distance between layers in the unit cell was tested. This was done by moving the other layer of the already optimized unit cell first 0.5 Å closer in the steps of 0.1 Å and 0.5 Å further away in the steps of 0.1 Å from the other layer. The cell parameters of the unit cell were not altered. NMR calculations were carried out for these systems using the same parameters as described above.

3.3. Defected systems

Different kinds of defected graphane systems were built. The starting geometries were created with Avogadro [63] from the optimized 1-layer models. The defects studied in this work were named G1, G2 and 2crenG where the G stands for graphene and numbers 1 and 2 for the number of concentric graphene rings in the middle of fully hydrogenated graphane. The cren-part in 2crenG means that the edge of the defect is crenelated like a

snowflake making it a bit bigger that G2-defect. Examples of the defected systems for the chair conformation are displayed in Figure 3.7, Figure 4.4 and in Figure 4.5. Rest of the systems are shown in Appendix B.

First the defect's effect on the hydrogenated carbon atoms were studied with different sized chair systems with G1 defects. The aim was to see how far the defects have to be from one another so that the values NMR shielding do not anymore noticeably change when going further away from one defect. Models were created by building 1-layer chair supercells where the unit cell of chair graphane was multiplied in the direction of the plane. The studied supercell sizes were 4×4×1, 5×5×1, 6×6×1, 7×7×1 and 8×8×1. The G1 defect was created by simply removing hydrogen atoms from the innermost concentric carbon ring.

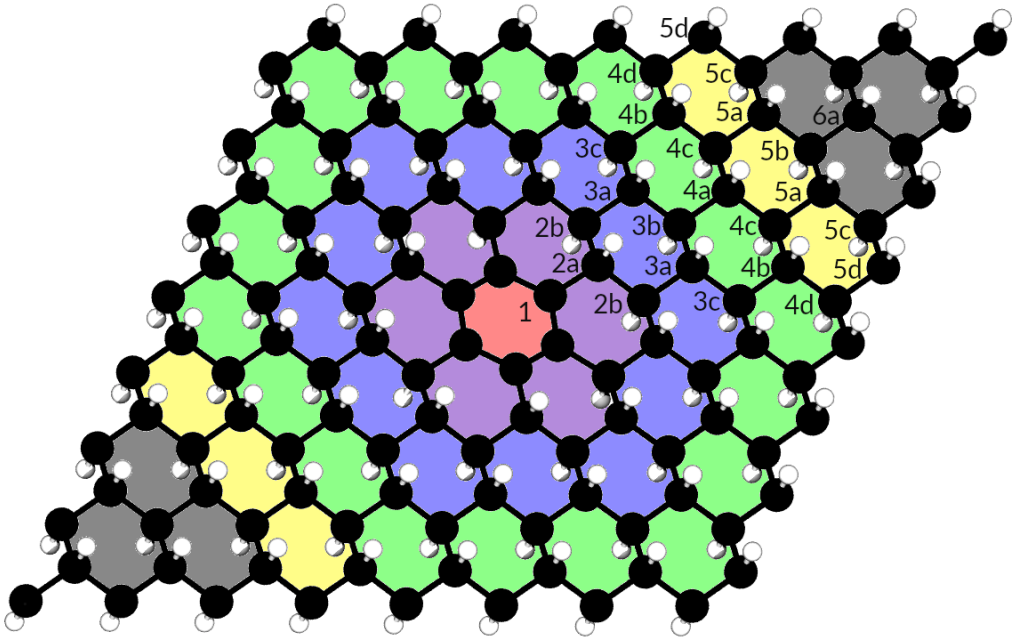

Figure 3.7: G1 defected $8 \times 8 \times 1$-sized chair supercell. Colors and numbers indicate different concentric rings. Letters indicate distance from the defect. Atom with label a is closest to the defect on that specific concentric ring, b is the second closest and so on forth.

The same converged parameters for cutoffs were used for the geometry optimizations and for the NMR calculations as for the pure systems. The k-point sampling was chosen to be $1 \times 1 \times 1$ due to the large unit cell resulting in dense k-point sampling in reciprocal space. The largest G1 system is displayed in Figure 3.7 with labeled carbon sites. Using the computed reference values of NMR shielding in methane, we can calculate the corresponding chemical shifts. These are presented in Table B.1 and the values are plotted in line charts in Figure 3.8 and in Figure 3.9 for supercells of each size.

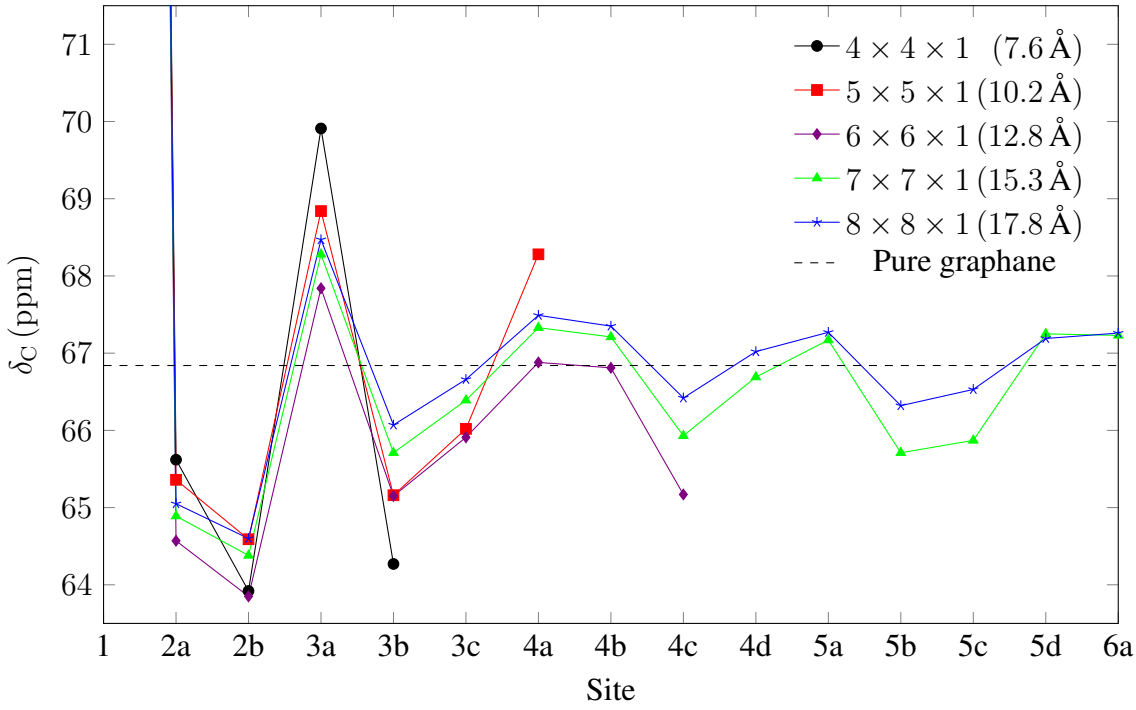

Figure 3.8: ^{13}C NMR chemical shifts in different-size G1-defected chair supercells. The distance between defects are indicated.

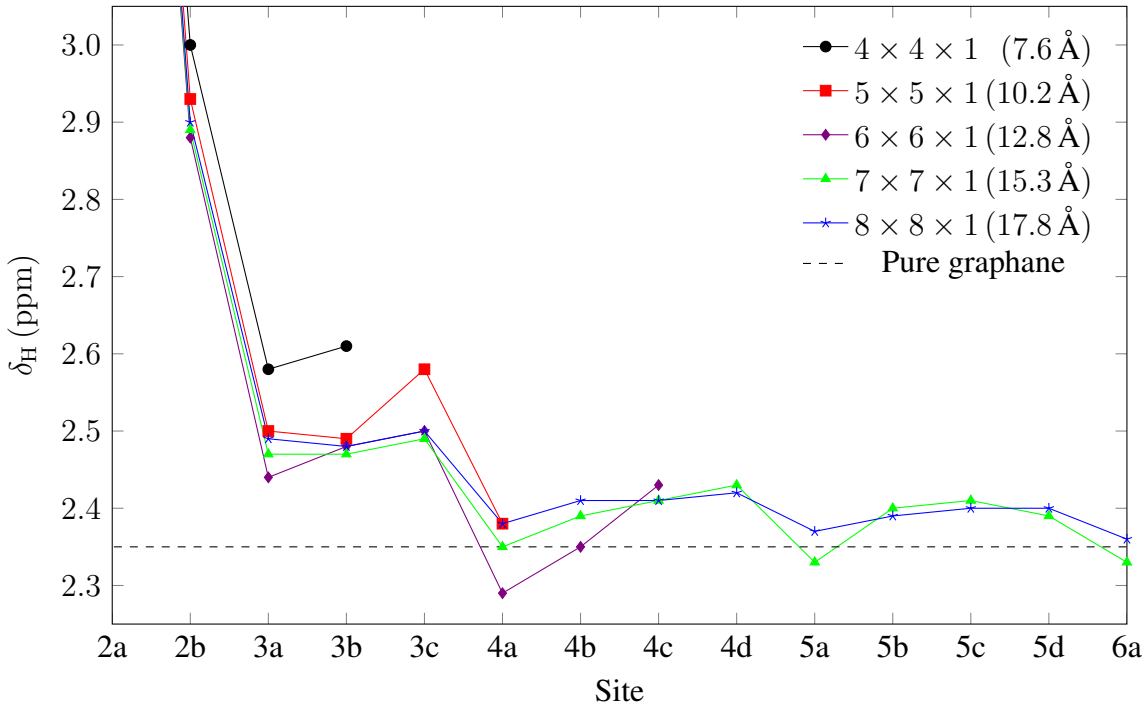

Figure 3.9: ^{1}H NMR chemical shifts in different-size G1-defected chair supercells. The distance between defects are indicated.

The used labeling puts carbon sites in the order of distance from the defect. However it should be noted that the distance according to labels is not linear. From Figure 3.8 we can see that the $6\times6\times1$, $7\times7\times1$ and $8\times8\times1$-sized, defected supercells produce very similarly shaped plots, which have a powerful oscillatory behavior near the defect and a weaker one near the edge. Similarly from Figure 3.9 we see that the ^{1}H chemical shifts start to converge around the same sites as the ^{13}C chemical shifts. The $6\times6\times1$ supercell, which has a distance of $12.7\,\text{Å}$ between the defects, was chosen to be the smallest converged system.

From the calculated NMR chemical shifts, it is also possible to simulate the spectrum. This was done by using MagresView 1.6.2 [75]. The ^{13}C spectra of the G1-defected systems are shown in Figure 3.10 with the spectrum of the pure 1-layered chair system for reference.

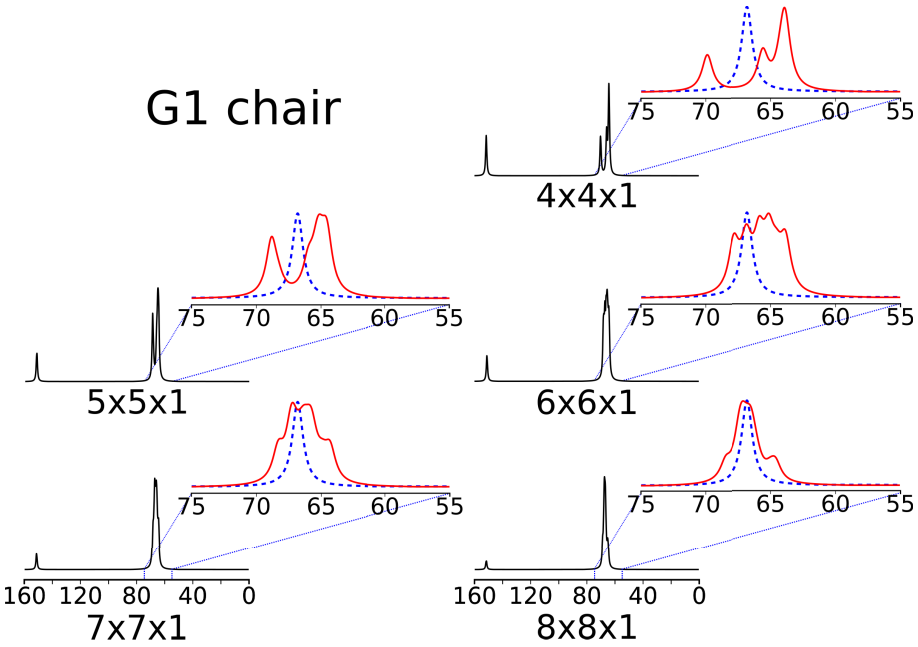

Figure 3.10: Lorentzian-broadened ^{13}C NMR chemical shift spectra of G1-defected different-size chair systems. The dashed blue spectrum is from the pure graphane (1-layered chair) system. Used line width is 0.5 ppm.

As noted, the $6 \times 6 \times 1$ supercell is big enough so that the chemical shifts of the hydrogenated carbon nuclei are close to the ones in the pure 1-layered chair system. This can also be seen from Figure 3.10. In the $5 \times 5 \times 1$ supercell there are only small number of nuclei that have a similar chemical shift compared to the pure graphane system. When the size is increased, the number of these nuclei also increases as there are more and more carbon sites that are close to the edge of the supercell. These sites resemble the pure graphane system as the defect is far away. Also the relative number of carbon atoms at the edge of defect decrease when the size of the system is increased. This is why the highest peak starts to look more like the sharp one of the pure systems and the peaks from the edge of the defect gets smaller when the supercell size is bigger. Also, it is worth noting that for the same reason the relative intensity of the peak from the defect carbon atoms at

around 150 ppm decreases when the supercell size increases.

Based on the tests, G2 and 2crenG-defected systems were built for all of the conformations. The systems were constructed so that the defect distance would be close to the value determined above. These values are shown in Table 3.4. The geometry optimization and NMR calculations were performed using the same parameters as for the G1 systems.

Table 3.4: Distances between defects in G2 and 2crenG-defected systems.

Conformation	G2	2crenG
chair	12.7 Å	15.2 Å
boat1	12.6 Å	10.1 Å
boat2	14.4 Å	10.1 Å
stirrup	12.8 Å	8.6 Å
twistboat	14.8 Å	10.4 Å
tricycle	15.3 Å	10.2 Å

Different geometric effects were observed from the optimized structures. These cause the systems to be unsymmetrical in some cases. This means that there are more inequivalent carbon sites, which leads to wider NMR chemical shift spectrum. For example, the 2crenG-defected chair supercell has a wavy edge as seen in Figure 3.11. Similar effect can also been seen for the 2crenG-defected boat-1, boat-2 and stirrup systems and for the G2-defected chair and stirrup systems. But, for example, in G2 twistboat system, the edge of the unit cell is like in the pure graphane system and there is no waviness.

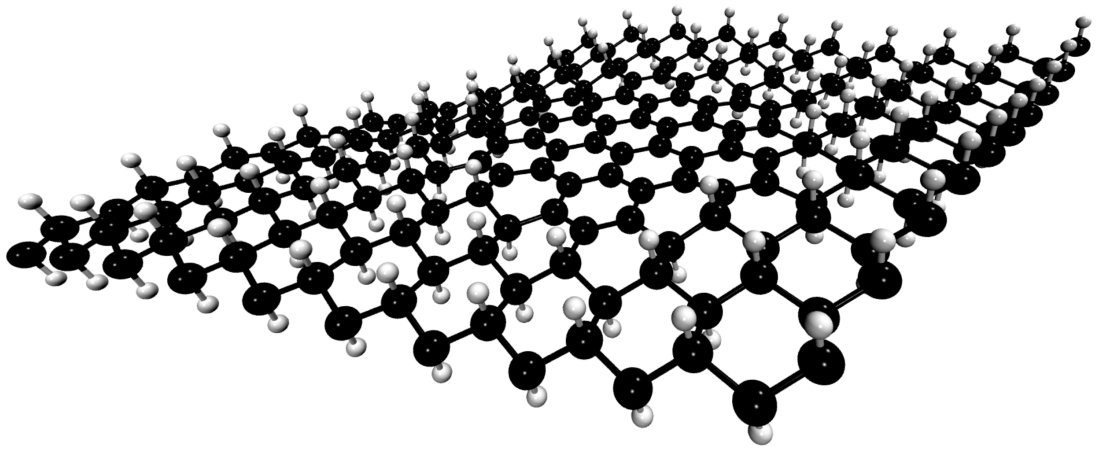

Figure 3.11: Defect causes waviness in the 2crenG-defected chair system. This can also be seen in 2crenG-defected systems for boat-1, boat-2 and stirrup and in the G2-defected chair and stirrup systems.

For the defected boat-2 systems in the optimized structures the defect forms a dent. This is displayed in Figure 3.12. Same sort of behavior is seen also in 2crenG boat-2 system. In the tricycle conformation in Figure 3.13, and also in the stirrup conformation, the defect is tilted and not aligned with the plane itself.

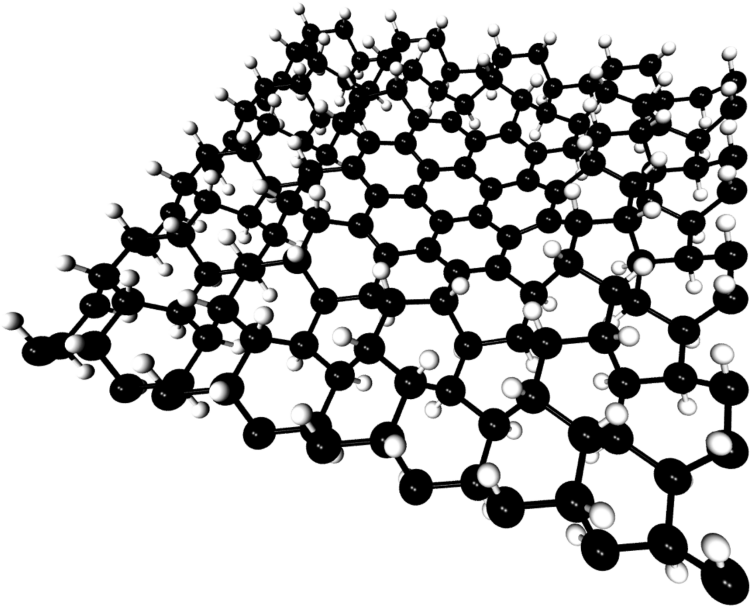

Figure 3.12: In the G2-defected boat-2 system the defect forms a dent in the plane. The same effect happens for the 2crenG-defected boat-2 system.

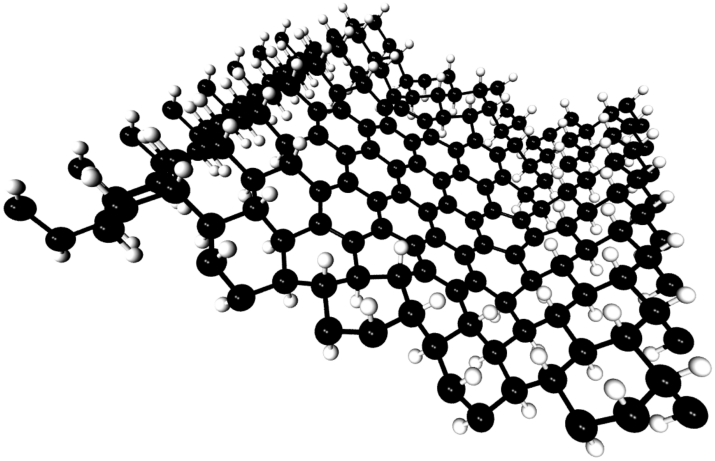

Figure 3.13: The defect is slightly tilted from the plane in the 2crenG-defected tricycle system. Similar behavior can be seen in all of the defected stirrup and tricycle systems.

4. Results and discussion

The results of this study are presented in this chapter. As described in the previous chapter the chemical shifts were calculated from the NMR shielding values using methane as a reference compound. The results are displayed here as Lorentzian-broadened NMR chemical shift spectra. All of the spectra of this study were made by using MagresView 1.6.2 [75]. The aim of these results is to provide a comprehensive computational insight into the chemical shifts of graphanes which can be used for example as a tool for analyzing experimental NMR spectra. All chemical shift values are displayed in Appendix A and Appendix B. The optimized geometries of the systems are presented in Appendix C.

4.1. Pure graphane systems

The ^{13}C and ^{1}H Lorentzian-broadened NMR spectra of the pure graphane systems are shown in Figure 4.1 and Figure 4.2. Computed values of chemical shifts are listed in Table A.1. Model pictures of the investigated graphane systems with labeled symmetry equivalent nuclear sites are shown for 1-, 2-, and 3-layer as well as bulk systems in Figure 3.6, Figure A.1, Figure A.2 and in Figure A.3 respectively.

From the ^{13}C spectra in Figure 4.1 it is possible to see that the conformations differ noticeably in chemical shifts but there is some overlap between them. Boat-2 conformation has the smallest chemical shift and chair has the largest. The same trend of chemical shifts between conformations applies regardless of the number of layers in the investigated system. For 1-layer systems there are only one or two distinct carbon sites which explain the simplicity of the spectra. However, for the many-layered systems there are more distinct sites and therefore the spectra have a more complex form. In Table A.1 there are presented for some sites in multi-layered systems a range of chemical shifts instead of one discrete value. This is due to subtle differences in relative geometries between atoms even though they represent the same symmetry-equivalent sites. For these systems chemical shifts are also overall larger and the largest values for sp^3-hybridized carbon atoms are obtained with the bulk systems.

For the chair conformation two types of stacking were used. From Figure 4.1 and from Figure 4.2 we can see that there are some differences between their spectra. For the 2-layered and bulk ab-stacked chair systems, there are two peaks instead of one. When there are two layers, the ab-stacked conformations have a slightly lower chemical shift but when we consider the bulk situation, the aa-stacked has the lower shift but only slightly.

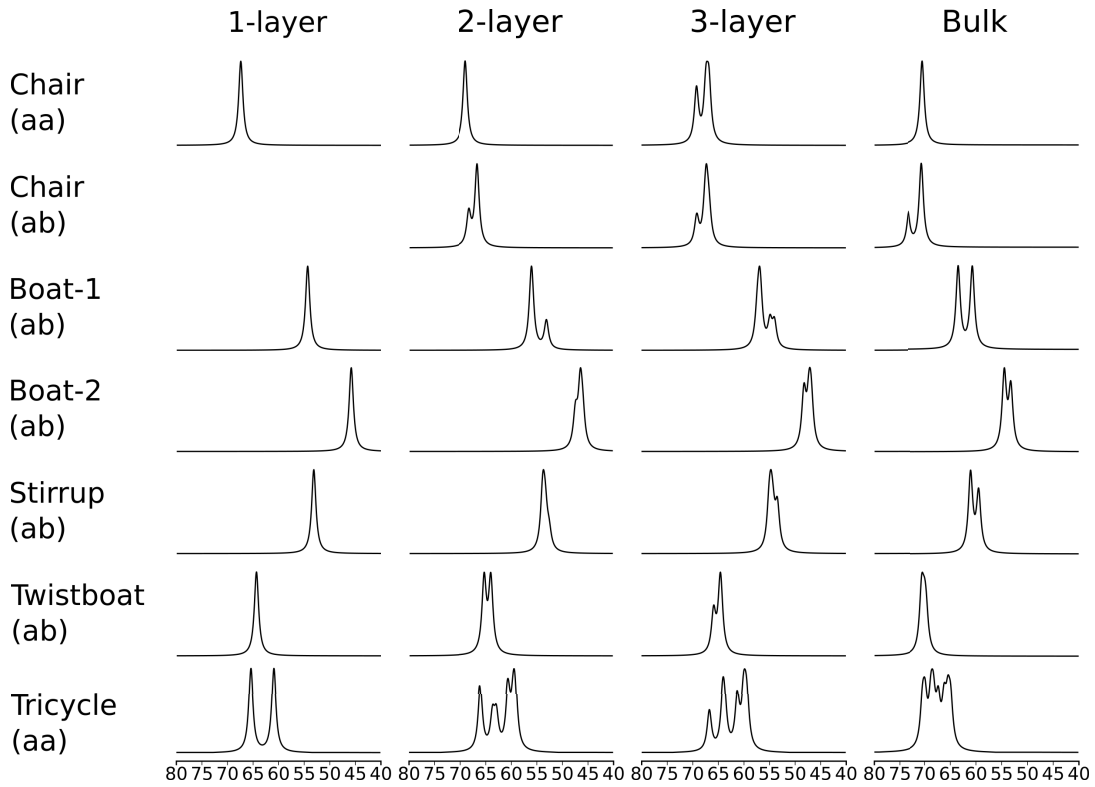

Figure 4.1: Lorentzian-broadened ^{13}C NMR chemical shift spectra of 1-layer, 2-layer, 3-layer and bulk systems for each conformation. Used line width is 0.5 ppm.

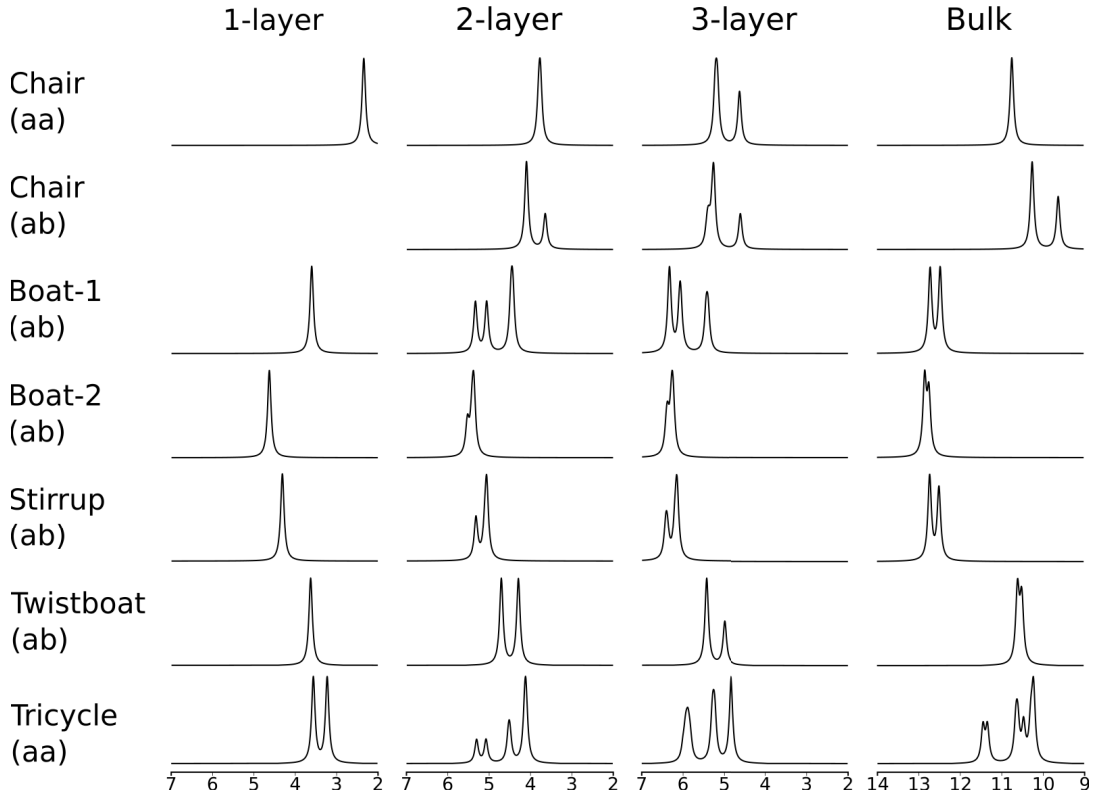

Figure 4.2: Lorentzian-broadened ^{1}H NMR chemical shift spectra of 1-layer, 2-layer, 3-layer and bulk systems for each conformation. Used line width is 0.05 ppm.

^{1}H NMR chemical shift spectra in Figure 4.2 shows also similar differences between conformations. For example, in the 1-layer systems all of the chemical shifts can be found between 2.35-4.63 ppm with some overlap between peaks. For the many-layered systems, the chemical shifts and the differences between them increase. The chemical shifts from the bulk systems are noticeably higher than from the others. Similar trends can still be observed as for the ^{13}C NMR chemical shift spectra. Overall the chemical shifts increase when there are more layers and the spectra become more complex due to higher number of distinct sites.

The 1-layer conformations can be arranged by their thermodynamic stability with the calculated Gibbs free energy [21]: Chair, Tricycle, Stirrup, Boat-1. Boat-2 and Twistboat, where Chair and Tricycle are the most stable conformations and the most probable ones to be synthesized. Because their chemical shifts are similar in different layered systems, their peaks would be likely to overlap in experimental samples and, due to their relatively high stability, they would be probably the ones with the highest intensities.

4.1.1. Changing layer distance in bulk systems

The distances d_l between layers of graphane in different optimized structures are also reported in Table A.1. Vishnyakova *et al.* [22] have experimentally determined layer distances by using high-resolution transmission electron microscopy (HRTEM) for graphane that has been synthesized from graphite. The value for threefold reduced graphite was reported to be 4.29 Å which is close to the value of aa-stacked bulk chair system (4.35 Å).

^{13}C and ^{1}H NMR chemical shifts for the bulk systems chair (aa) and chair (ab) as a function of change in layer distance are shown in Figure 4.3. The computed values of NMR chemical shifts are presented in Table A.2. When the distance is increased the chemical shift of one site increases and the chemical shift of the other site decreases. This goes the opposite way around when the distance is changed in the other direction. Overall, we observe a symmetric behaviour for the chemical shifts, which is expected. Moving the layers in one unit cell closer to one another is the same as moving them further apart as the layer from the next unit cell will become closer. This is due to the unaltered unit cell height.

For the aa-stacked system we see that there are no differences between sites A and B when the layer distance is at its optimized value. When we change it, the sites become inequivalent and they have different chemical shifts. For the ab-stacked system the sites are already inequivalent for the optimized layer distance. When it is increased, we reach a point where the sites become equivalent and therefore they have same chemical shifts, which is at $72.00\,\mathrm{ppm}$ for ^{13}C. For comparison, the 1-layer chair has a chemical shift of $\delta_{\mathrm{C}} = 66.84\,\mathrm{ppm}$.

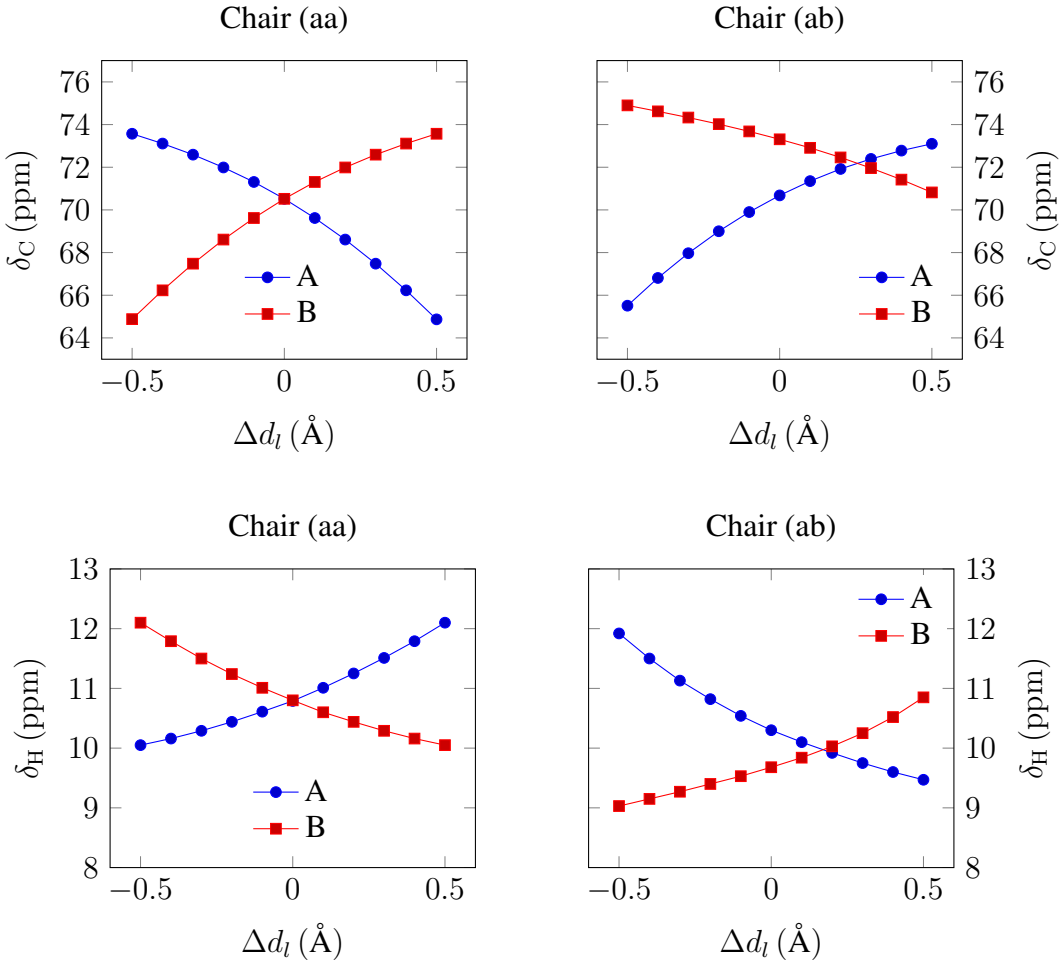

Figure 4.3: ^{13}C and ^{1}H NMR chemical shifts (δ_C and δ_H in ppm) for bulk systems chair (aa) and chair (ab) as a function of change in layer distance (Δd_l in Å). The zero value for the change in layer distance corresponds to the optimized geometry for the specific bulk system.

4.1.2. Comparison to other computational studies

As stated earlier, the only computed NMR shieldings in the case of graphane with periodic methods exist for the 1-layer chair system. Hence it is the only system that we can reliably compare to other computational studies by chemical shifts. Vähäkangas *et al.* [27] computed the NMR shieldings for the chair system: $\sigma_C = 121.89\,\text{ppm}$ and $\sigma_H = 30.66\,\text{ppm}$. In this study the corresponding values are computed to be $\sigma_C = 120.22\,\text{ppm}$ and $\sigma_H = 28.50\,\text{ppm}$. So, there is an approximately 2 ppm difference between the results.

Because Vähäkangas *et al.* used a smaller k-point density, more test calculations were performed for 1-layer chair and boat-2 conformations to ensure that the used k-point grids were dense enough. These two conformations were used because chair has the biggest and boat-2 the smallest chemical shift from studied conformations. For the test calculations the k-points were doubled in every direction. The results did not change from the original calculation, so the used sampling was dense enough. Therefore, we can conclude that the

difference in shielding does not come from the used *k*-point sampling.

The difference also cannot be explained by the cutoff energy because in this study the value was higher and clearly converged. Also, additional tests were performed using even higher cutoffs (150 Ry and 200 Ry) and no changes were observed. A possible source that could make the difference is the used pseudopotential. In both cases the used pseudopotential was a US-pseudopotential. It is however impossible to be sure because the exact pseudopotential file used by Vähäkangas *et al.* is unknown.

Vähäkangas *et al.* also computed the values for NMR shielding using the cluster method. This was done also by Özcan *et al.* [49]. These values are shown in Table 4.1. In both cases the cluster method was used with different sized graphane clusters. The naming convention is the same as the one used in this thesis for the graphene defects. Now for example the HG3 stands for cluster of hydrographene (HG) *ie.* graphane cluster which has three concentric carbon rings. As we can see from Table 4.1 the values achieved using the cluster approach are higher than the ones obtained with periodic methods with the largest used cluster sizes. By comparing the values computed by Özcan *et al.* [49] with different exchange and correlation functionals we can see that it alone can affect the results by 5 ppm.

Table 4.1: Computed values of σ_{C} and σ_{H} (ppm) for the chair conformation with cluster and periodic methods from previous studies. In this study the corresponding values are computed to be $\sigma_{\mathrm{C}} = 120.22\,\mathrm{ppm}$ and $\sigma_{\mathrm{H}} = 28.50\,\mathrm{ppm}$.

	System							
	HG1	HG2	HG3	HG4	HG5	2crenHG	3crenHG	Periodic
$\sigma_{\mathrm{C}}{}^{a}$ [27]	145.81	121.38	123.13	123.22	-	-	-	121.89
$\sigma_{\mathrm{H}}{}^{a}$ [27]	29.86	30.6	30.5	30.53	-	-	-	30.66
$\sigma_{\mathrm{C}}{}^{b}$ [27]	143.94	122.04	123.68	123.22	-	-	-	-
$\sigma_{\mathrm{H}}{}^{b}$ [27]	29.79	30.64	30.56	30.59	-	-	-	-
$\sigma_{\mathrm{C}}{}^{c}$ [49]	148.38	122.93	124.61	124.70	124.93	124.12	124.91	-
$\sigma_{\mathrm{C}}{}^{d}$ [49]	151.82	128.18	129.7	129.73	129.8	129.21	130.01	-

[a] The geometry was optimized as cluster (relax). [b] The geometry of the periodic system was used (fixed). [c] The used exchange and correlation functional was the B3LYP functional. [d] The used exchange and correlation functional was the BHandHLYP functional.

4.2. Defected systems

In addition to different-size G1-defected chair systems, the NMR chemical shifts were determined for G2 and 2crenG-defected graphane systems with different conformations. An example of a G2-defected system is shown in Figure 4.4 and, similarly, an example of a 2crenG-defected system is shown in Figure 4.5. Rest of the G2 and 2crenG-defected systems are displayed in Appendix B.

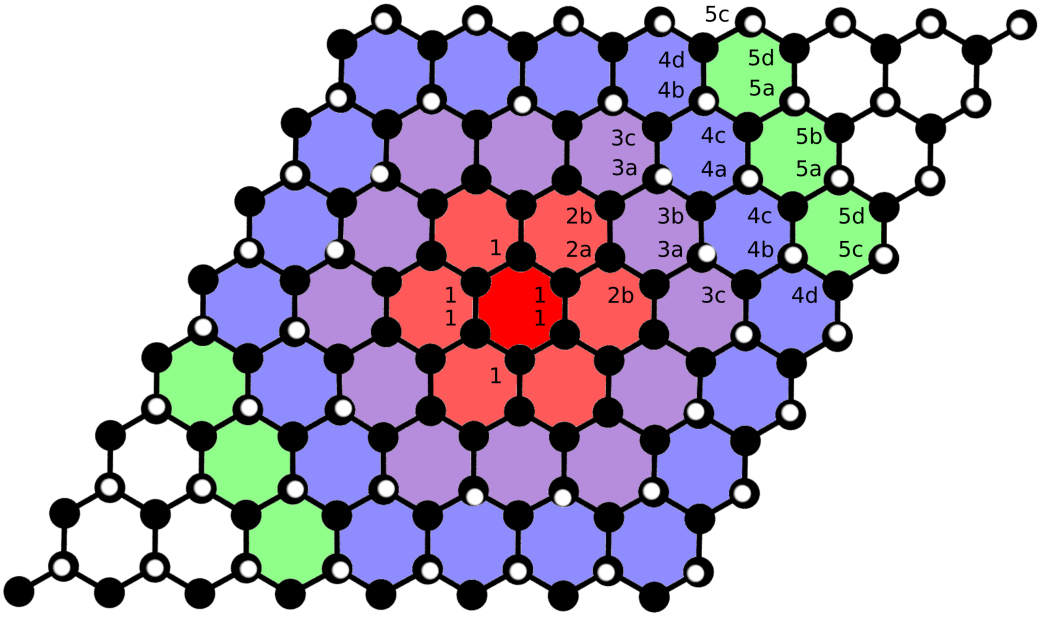

Figure 4.4: G2-defected chair supercell. Labeling according to figure 3.7. The G2-defect is colored red.

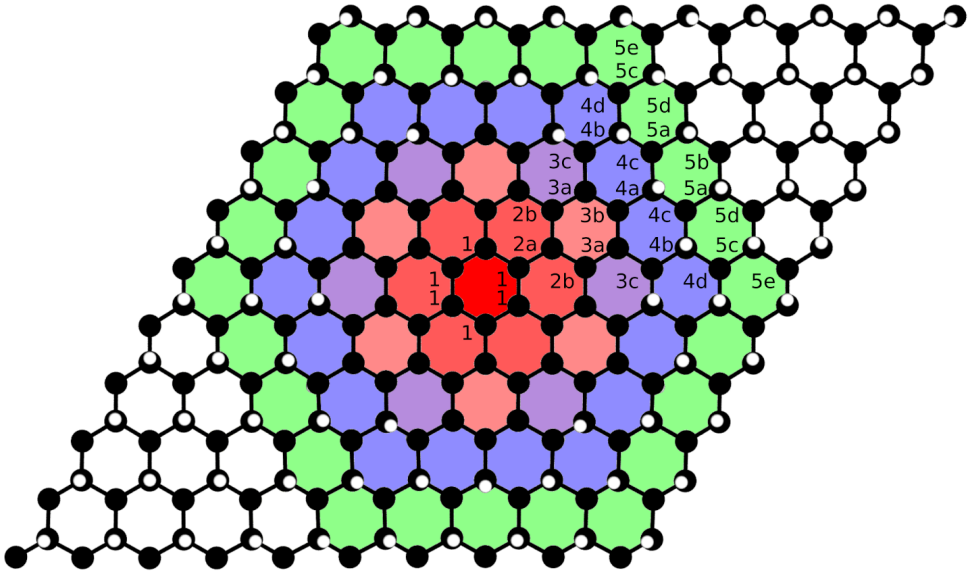

Figure 4.5: 2crenG-defected chair supercell. Labeling according to figure 3.7. The 2crenG-defect is colored red.

All of the computed values for the ^{13}C and ^{1}H NMR chemical shifts are found in Appendix B. In them there is a 4-step labeling scheme for different symmetry equivalent nuclear sites. For example in Figure B.8 there is a site labeled *A3c2* where *A* tells the closest carbon in the centermost concentric carbon ring, *3* tells the number of the concentric carbon ring where the site is, *c* tells that the site is third-closest to the center of the

system among the sites on that ring, and *2* tells that it is the second nonequivalent site on that same ring at the same distance from the center. For some conformations every carbon in the innermost ring is symmetry equivalent and only one sixth of the system is needed to be labeled as the other ones are symmetrical and therefore the chemical shifts are the same. Therefore, for example in Figure 4.4, there is no capital letter in the labeling. On the other hand, some conformations have less symmetry and they hold more symmetrically nonequivalent sites and labeling from *A* to *F* is needed. This can also be seen in Figure 3.11, Figure 3.12 and in Figure 3.13.

The Lorentzian-broadened ^{13}C NMR chemical shift spectra of G2 and 2crenG-defected systems are shown in Figure 4.6. The pure graphane spectra of the corresponding conformation is also shown for reference with dashed blue lines. The peaks from the defect (130-170 ppm) and from the graphane parts (40-80 ppm) are also shown more closely.

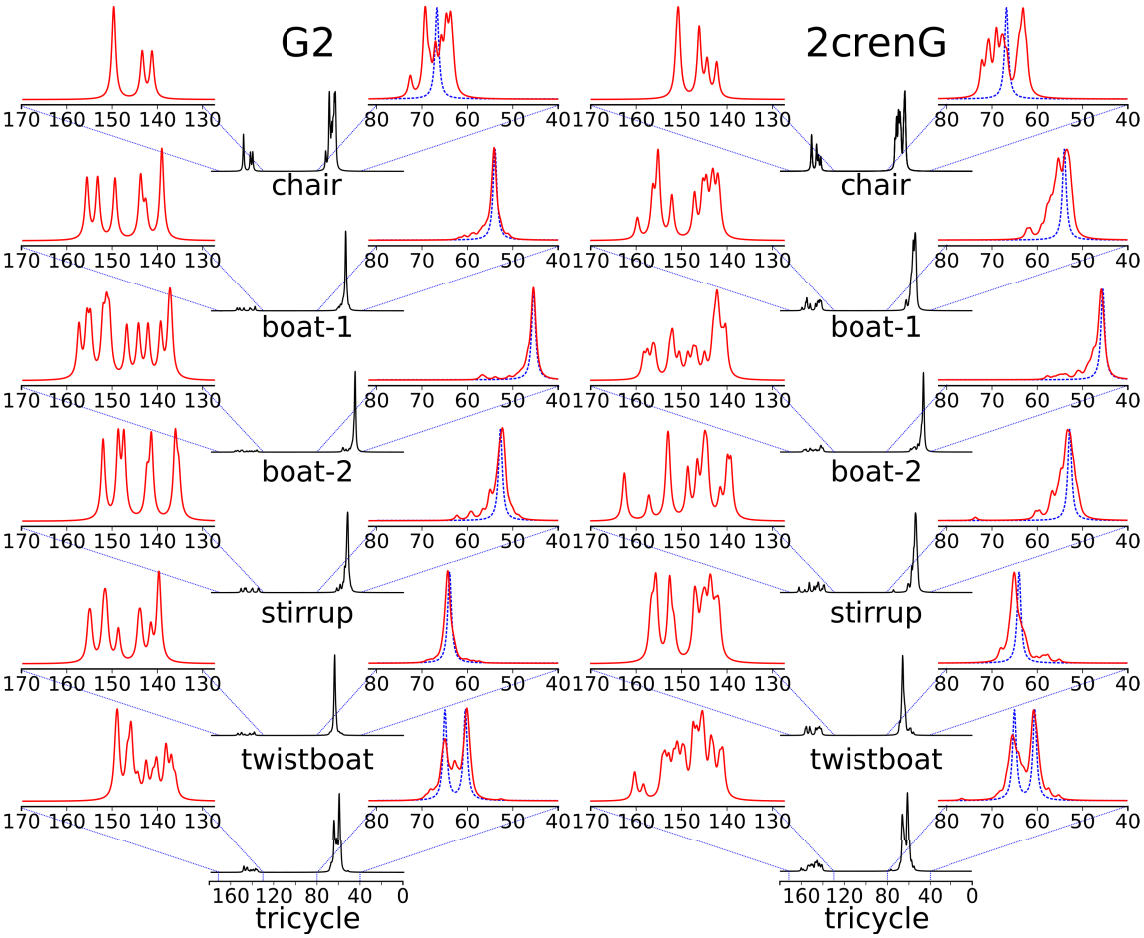

Figure 4.6: Lorentzian-broadened ^{13}C NMR chemical shift spectra of G2 and 2crenG-defected systems. The dashed blue spectrum is from the corresponding 1-layered pure graphane system. Used linewidth is 0.5 ppm.

It can be seen from Figure 4.6 that for the most parts the hydrogenated peaks are pretty similar to the ones of the pure graphane system. In general, they are wider for the defected systems. It can also be seen that the peaks from hydrogenated carbon atoms differ between conformations in similar manner that they did in the pure graphane systems. The biggest differences can be seen for the defected chair systems where the peaks are spread widely around the peak of the 1-layered pure graphane chair. Similar behaviour is seen for the 5×5×1-sized G1-defected chair system in Figure 3.10. The fact that the peaks from hydrogenated carbon atoms are close to the corresponding value of the pure graphane systems also tells that the size of the supercell is big enough so that the value of chemical shift near the edge of the unit cell is similar to the value of it in the pure system. The peaks of the hydrogenated carbons in Figure 4.6 do not differ noticeably between the G2 and 2crenG-systems except for the chair conformation. The values of chemical shifts between the highest peaks are practically same with G2 and 2crenG-defects. However, when the defect is 2crenG, the spectra are wider and more complex.

The peaks from the defect are small in intensity due to its small size compared to the size of the whole system. Also, they are spread widely around 135 ppm - 165 ppm and differ noticeably for the different conformations. For example, the chair conformation with the G2-defect has only three peaks but the G2-defected boat-2 system has at least eight noticeable ones. With different conformations the geometry around the defect is different as seen for example in Figure 3.11, Figure 3.12 and in Figure 3.13. This also affects the electronic structure of the system and this explains the differences between conformations. Similar effects have been reported by Özcan *et al.* [49]. When comparing the peaks form the defect between the G2 and 2crenG-defected systems, we see that the spectra of the 2crenG-defected system have a more complex form. This can be explained by the size and shape of the 2crenG-defect compared to the G2-defect. With the 2crenG-defect, there are more sites at the edge of the defect.

The ^{1}H NMR chemical shift spectra of defected systems are shown in Figure 4.7. Computed values for these chemical shifts can also be found in Appendix B. From the spectra it is easy to see a trend, where the defected peaks are significantly shifted to the left. Similar behavior of chemical shifts between conformations is seen here as it can be seen for the ^{13}C spectra. The relative positions of peaks from different conformations compared to each other stay the same regardless of the presence or size of the defect.

When comparing the ^{1}H NMR chemical shift spectra of different-size G1-defected systems, we see again a similar trend compared to the corresponding ^{13}C spectra. For the smallest system (4×4×1) there are more values of chemical shifts with relatively high intensities, but when the size of the system is increased, the spectra obtain a simpler form. Again, this is a consequence from the fact that there are now more protons at the edges of the system, where it resembles the pure 1-layer graphane chair system.

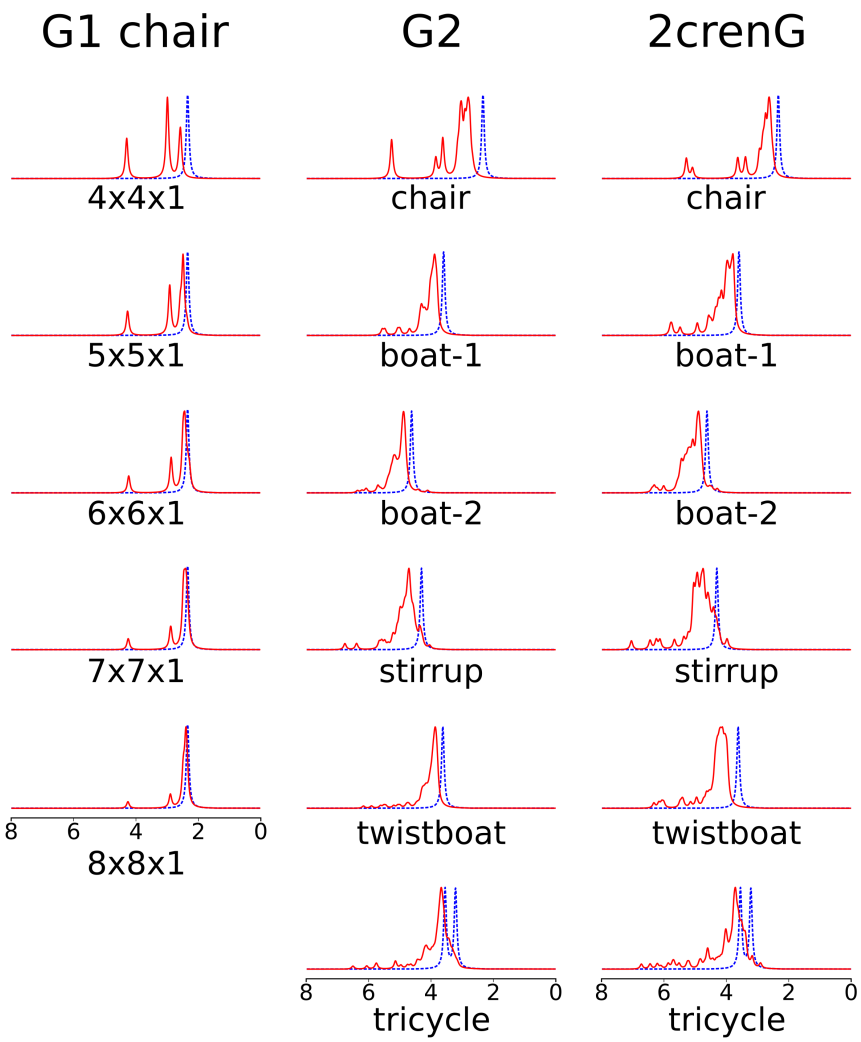

Figure 4.7: Lorentzian-broadened ^{1}H NMR chemical shift spectra of defected systems. Used line width is 0.05 ppm [75].

4.2.1. Comparison to experimental study

As noted earlier, Vishnyakova *et al.* [23] hydrogenated commercial graphite using $\mathrm{Li/NH_3}$ as the reducing agent and tert-butyl alcohol as a proton source. The reduction was done three times and NMR spectroscopy was used after the reductions to investigate the product. This was done by solid state NMR spectroscopy measuring ^{1}H-^{13}C cross polarization magic angle spinning (CPMAS) spectrum and also direct ^{13}C MAS spectrum. Based on the carried out analysis they concluded that there appears to be interior benzene rings surrounded by hydrogenated graphene i.e. graphane. Comparing the experimental results to the ones computed by Vähäkangas *et al.* [27] and Özcan *et al.* [49] they fortified this conclusion. However, in these computational studies only the chair conformation was studied.

Based on the computed ^{13}C NMR chemical shifts presented here we can also verify this conclusion. Figure 4.8 shows the experimental center band region of MAS, direct ^{13}C pulse (90°) spectrum of the synthesized product which is thought to be graphane with

interior benzene rings. According to Vishnyakova *et al.* the intensities of the peaks from the defects and from the hydrogenated areas are not comparable. However qualitatively the spectrum looks similar to the ones displayed here.

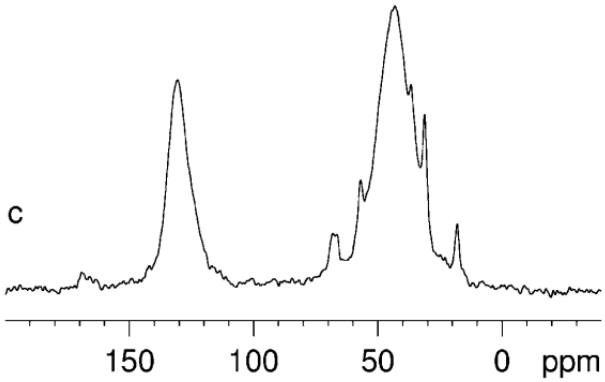

Figure 4.8: Center band region of MAS direct ^{13}C pulse (90°) spectrum of three times reduced graphite using relaxation delay of 300 s. Printed with permission from [22]. Copyright (2016) Wiley.

In Figure 4.8 there are also peaks from the used solvents. According to Vishnyakova *et al.* the peaks at about 67 and 31 ppm are from residual tert-butyl alcohol and the peaks at about 57 and 18 ppm are from residual ethanol. The highest intensity of the peak from the hydrogenated carbons is observed at around 43 ppm and similarly the highest intensity from the defected area is observed at about 131 ppm. Therefore, the difference of these peaks is 88 ppm. From the G1-defected chair ^{13}C spectra in Figure 3.10 we can see that when the defects are close to one another, as in the $4\times4\times1$ sized system, the difference between the peak from the defect and from the highest peak of the hydrogenated carbons is close to the value of 88 ppm. When the size of the system is increased the difference decreases slightly. For the $8\times8\times1$ sized system the difference is close to 84 ppm. For the G2-defected chair the peaks from the defect and also from the hydrogenated carbons spread to a wider area but the difference between them does not change noticeably. Same applies also for the 2crenG chair system.

As noted earlier the ^{13}C chemical shifts differ between different conformations in the hydrogenated areas but not significantly in the defect. In G2 and 2crenG-defected systems the lowest values of ^{13}C chemical shifts are obtained when using the boat-2 conformation at about 45 ppm and the highest values are obtained with the chair conformation at about 70 ppm. There is therefore a range with a width of about 25 ppm where the peaks from different conformations can be found when there is either G2 or 2crenG-defect.

For conformations such as boat-2 , boat-1 and stirrup, which have small ^{13}C chemical shifts in the defected systems, the difference of hydrogenated and defect peaks is closer to 100 ppm, which is larger than the one in the spectrum measured by Vishnyakova *et al.* in Figure 4.8. These conformations are also more unlikely to be synthesized according to their Gibbs free energy as noted by He *et al.* [21]. However, the peak from the hydrogenated carbons in the experimental spectra is also wide even when considering the

solvents. Nevertheless, there is room for speculation that the sample measured by Vishnyakova *et al.* consists of mostly chair and tricycle conformations as they are the most likely ones to be synthesized. The computational spectra represented here are more similar to the experimental ones when considering just these conformations but also the main peaks from the other conformations overlap with the experimental spectra.

5. Conclusions

The theoretical background for this computational NMR study of periodic graphane systems was built on density functional theory (DFT) and the gauge-including projector augmented wave (GIPAW) method. The main principles of these theoretical methods were presented. With these theories the NMR chemical shifts for graphane in different conformations were calculated using Quantum Espresso which is an open source computer code for electronic-structure calculations and materials modeling.

The computational parameters, such as cutoff energies and the sizes of *k*-point sampling, were carefully evaluated before the actual calculations to be sure of the accuracy of the computations with a reasonable computational cost. With these parameters the geometries of the investigated systems were optimized to relaxed structures. For these the values of NMR shielding and thereby the values for chemical shifts were determined for both $^{13}\mathrm{C}$ and $^{1}\mathrm{H}$ nuclei.

Computations were performed for pure graphane 1-layered, 2-layered, 3-layered and bulk systems and graphene defected systems. This is the first time that the values for NMR shielding are computed for all six conformations of graphane in different layered systems. It was shown that the $^{13}\mathrm{C}$ and the $^{1}\mathrm{H}$ NMR chemical shift spectra differ noticeably for the different conformations in all of the different systems. The number of layers also affects the spectra but not as much as the conformations do. By comparing the results to a previous study made for the 1-layered chair [27], it was noticed that the results differed by close to 2 ppm. The most probable source of this difference is the used pseudopotential.

Experimental spectrum was analyzed qualitatively based on the computed spectra of the graphene-defected systems. It was seen that the spectra had many similarities. The overall shape of them looked similar and the distances between graphane and graphene peaks were similar. This demonstrates the importance of computational NMR values. It allows a more detailed analysis of an experimental spectra.

In this study for the G1 defect, only the chair conformation was considered. This could also be done for the other conformations like it was done with the G2 and 2crenG graphene-defected systems. One possibility would also be to investigate systems with bigger defects. Based on the study by Vishnyakova *et al.* [23] it would be interesting to into account the left-over solvent molecules between the graphene-defected graphane layers.

The only NMR parameter considered in this study was the NMR shielding. It is also possible to determine the coupling constant of the indirect spin-spin coupling. This has been done for graphane only using the chair conformation [27, 49]. Also, the func-

tionalization of graphene can also be done with other compounds than hydrogen. For example, fluoridated graphene *ie.* fluorographene is one possibility. The computed NMR parameters for it exist also only for the chair conformation [27, 49] so a more general computational study would be in demand.

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A. Pure graphane systems

Table A.1: NMR chemical shifts for ^{13}C and ^{1}H (δ_C and δ_H in ppm) in pure graphane 1-layer, 2-layer, 3-layer and bulk systems. Pictures of investigated systems and labeled sites are shown in Figure 3.6, Figure A.1, Figure A.2 and Figure A.3. For some sites there are multiple values of NMR chemical shifts. The smallest and biggest values are presented. The distances between layers d_l are presented in Å for the multi-layered systems.

	Site		Chair (aa)	Chair (ab)	Boat-1	Boat-2	Stirrup	Twistboat	Tricycle
1-layer	δ_C	A	66.84	-	53.76	45.26	52.19	64.07	64.91
		B	-	-	-	-	-	-	60.10
	δ_H	A	2.35	-	3.57	4.63	4.38	3.61	3.36
		B	-	-	-	-	-	-	3.49
2-layer	δ_C	A	68.61	67.84	55.56	46.09	53.26	64.82-64.88	65.68-65.72
		B	68.52	66.24	55.71	46.06	52.93	63.53-63.60	58.86-59.11
		C	-	-	55.52	45.62	53.41	-	60.07-60.32
		D	-	-	52.69	47.03	52.16	-	62.58-63.27
	δ_H	A	3.81	3.65	4.44	5.38	5.07	4.30	4.14
		B	3.85	4.11	4.48	5.38	5.07	4.72	4.50-4.53
		C	-	-	5.34	5.42	5.33	-	4.11
		D	-	-	5.07	5.53	5.11	-	5.03-5.31
	d_l		5.88	4.37	4.22	4.85	4.76	4.61	5.18
3-layer	δ_C	A	68.89	68.89	56.67	46.93	53.95	65.54-65.56	66.32-66.50
		B	66.47	66.64	56.54	46.90	54.30	64.13	59.48-59.76
		C	67.04	67.36	56.36	46.44	54.40	64.31	60.78-61.04
		D	-	67.07	53.69	47.84	53.09	-	63.25-63.77
		E	-	-	57.01-57.06	47.94-47.96	54.70-54.74	-	63.39-63.84
		F	-	-	54.53-54-56	46.57	53.11-53.14	-	58.99-59.25
	δ_H	A	4.63	4.61	5.45	6.26	6.15	5.00	4.85
		B	5.23	6.43	5.41	6.25	6.15	5.43	4.25
		C	5.18	6.39	6.35	6.29	6.42	5.44	4.82
		D	-	5.27	6.06	6.41	6.20	-	5.88-6.00
		E	-	-	6.33	6.38	6.39	-	5.82-5.94
		F	-	-	6.09	6.28	6.17	-	5.28-5.30
	d_l		4.72	4.72	4.23	4.85	4.75	4.59	5.18
Bulk	δ_C	A	70.15	72.93	60.37-60.44	52.91	60.74	69.34-70.25	67.89-70.04
		B	-	70.30	63.13-63.15	54.17	59.15	-	64.52-66.96
	δ_H	A	10.75	9.63	12.48	12.75	12.73	10.50-10.62	10.23-11.45
		B	-	10.25	12.72	12.85	12.51	-	10.24-10.66
	d_l		4.35	4.45	4.16	4.87	4.76	4.69	5.17

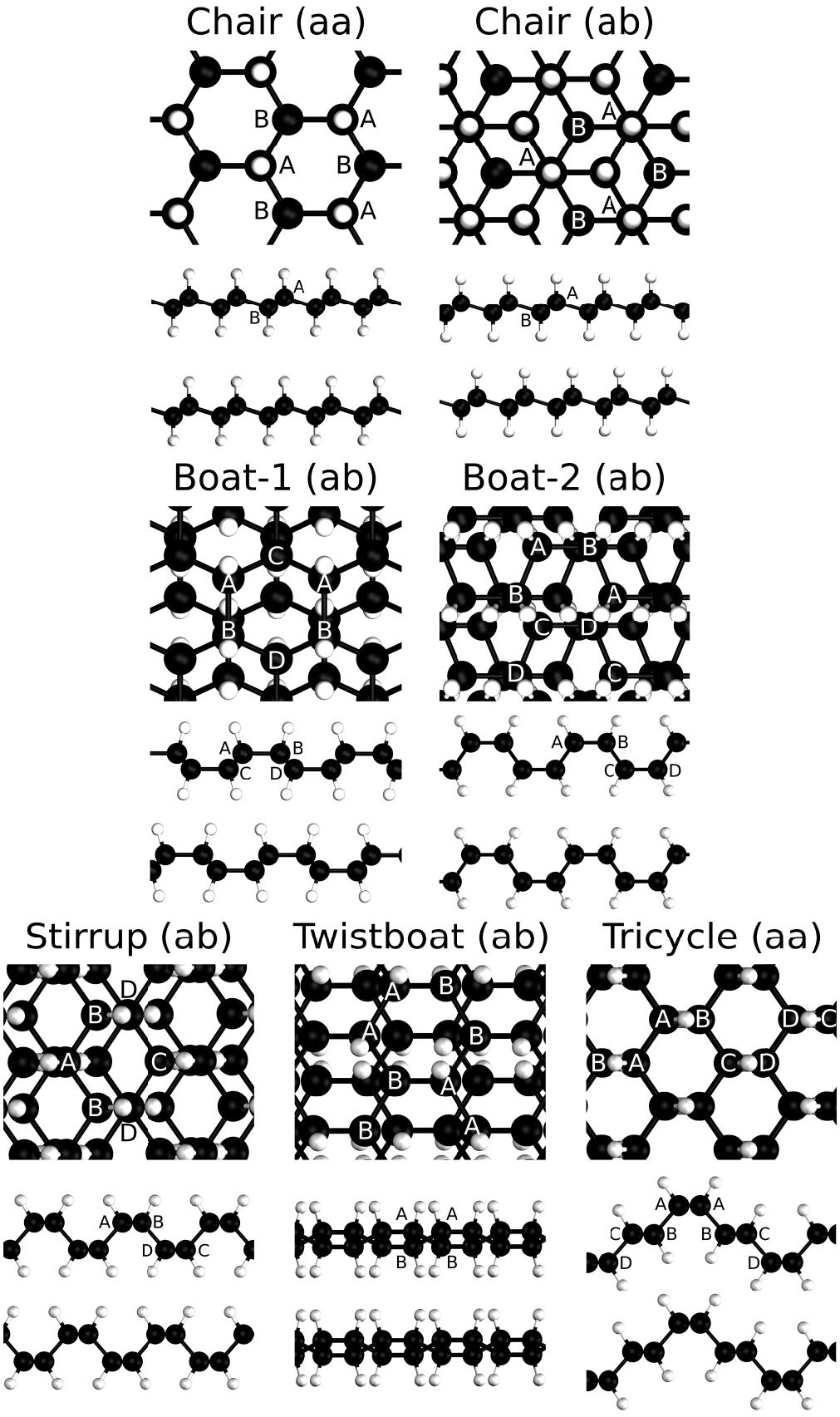

Figure A.1: 2-layered systems. Distinct carbon sites are indicated with capital letters. Both layers in each system are equivalent due to symmetry.

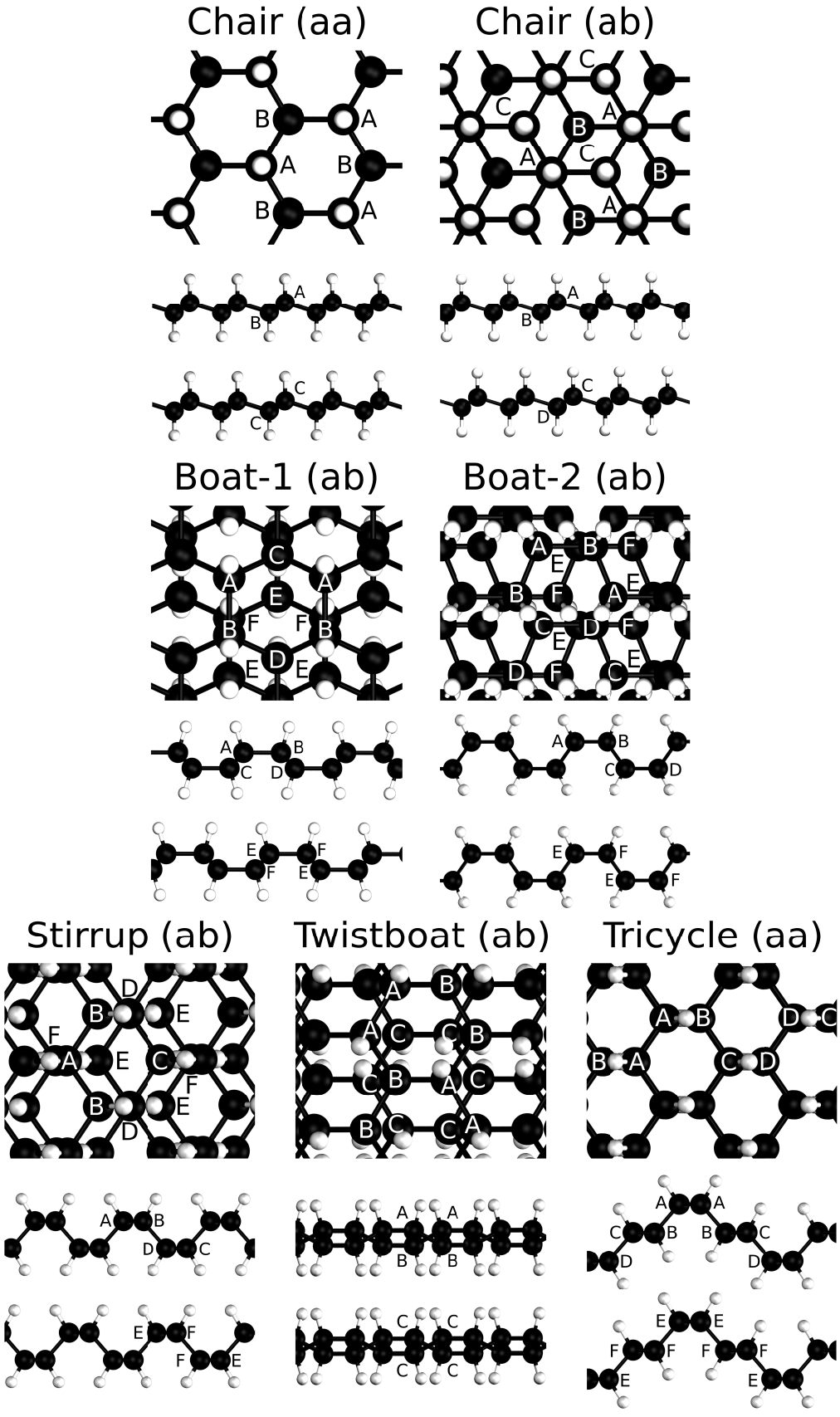

Figure A.2: 3-layered systems. Distinct carbon sites are indicated with capital letters. Only the inner and one outer layer are shown. The other outer layer can be regarded as equivalent to the shown upper layer.

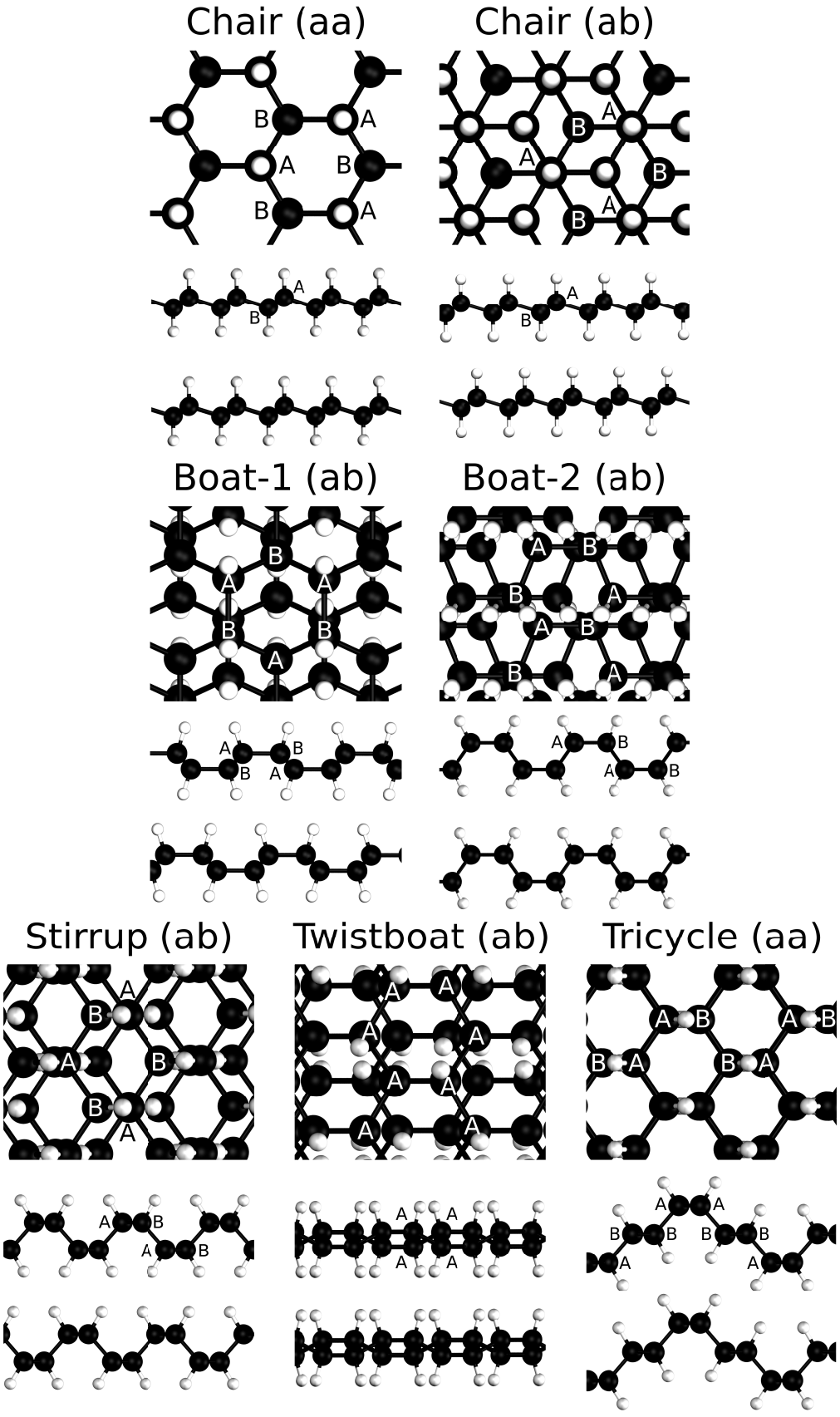

Figure A.3: Bulk systems. Distinct carbon sites are indicated with capital letters.

Table A.2: Values for NMR chemical shifts (δ_{C} and δ_{H} in ppm) for $^{13}\mathrm{C}$ and $^{1}\mathrm{H}$ in chair (aa) and chair (ab) bulk systems where the distance between layers is manually altered (Δd_l in Å). Values of this table are plotted in figure Figure 4.3.

	Δd_l (Å)		-0.5	-0.4	-0.3	-0.2	-0.1	0	0.1	0.2	0.3	0.4	0.5
Chair (aa)	δ_{C}	A	64.51	65.86	67.11	68.24	69.25	70.15	70.94	71.62	72.22	72.74	73.20
		B	73.20	72.74	72.22	71.62	70.94	70.15	69.25	68.24	67.11	65.86	64.50
	δ_{H}	A	12.05	11.74	11.45	11.19	10.96	10.75	10.55	10.39	10.24	10.11	10.00
		B	10.00	10.11	10.24	10.39	10.56	10.74	10.96	11.20	11.46	11.74	12.05
Chair (ab)	δ_{C}	A	74.53	74.25	73.96	73.65	73.31	72.94	72.54	72.09	71.59	71.05	70.45
		B	65.14	66.44	67.60	68.63	69.53	70.31	70.98	71.55	72.02	72.41	72.73
	δ_{H}	A	11.87	11.45	11.08	10.77	10.49	10.25	10.05	9.87	9.70	9.55	9.42
		B	8.98	9.10	9.22	9.35	9.48	9.63	9.79	9.98	10.20	10.47	10.80

B. Defected systems

Table B.1: Calculated $^{13}\mathrm{C}$ and $^{1}\mathrm{H}$ NMR chemical shifts ($\delta_{\mathrm{C}}\,(\mathrm{ppm})$ and $\delta_{\mathrm{H}}\,(\mathrm{ppm})$) for different sized G1-defected chair systems.

		Supercell size				
	Site	$4\times4\times1$	$5\times5\times1$	$6\times6\times1$	$7\times7\times1$	$8\times8\times1$
δ_{C}	1	151.25	151.38	150.74	151.14	151.40
	2a	65.62	65.36	64.57	64.89	65.05
	2b	63.92	64.59	63.85	64.38	64.60
	3a	69.91	68.84	67.84	68.28	68.47
	3b	64.27	65.16	65.15	65.71	66.07
	3c	-	66.02	65.91	66.39	66.66
	4a	-	68.28	66.88	67.33	67.49
	4b	-	-	66.81	67.21	67.35
	4c	-	-	65.17	65.93	66.42
	4d	-	-	-	66.69	67.02
	5a	-	-	-	67.17	67.27
	5b	-	-	-	65.71	66.32
	5c	-	-	-	65.87	66.53
	5d	-	-	-	67.25	67.19
	6a	-	-	-	67.23	67.26
δ_{H}	1	-	-	-	-	-
	2a	4.30	4.27	4.24	4.25	4.26
	2b	3.00	2.93	2.88	2.89	2.90
	3a	2.58	2.50	2.44	2.47	2.49
	3b	2.61	2.49	2.48	2.47	2.48
	3c	-	2.58	2.50	2.49	2.50
	4a	-	2.38	2.29	2.35	2.38
	4b	-	-	2.35	2.39	2.41
	4c	-	-	2.43	2.41	2.41
	4d	-	-	-	2.43	2.42
	5a	-	-	-	2.33	2.37
	5b	-	-	-	2.40	2.39
	5c	-	-	-	2.41	2.40
	5d	-	-	-	2.39	2.40
	6a	-	-	-	2.33	2.36

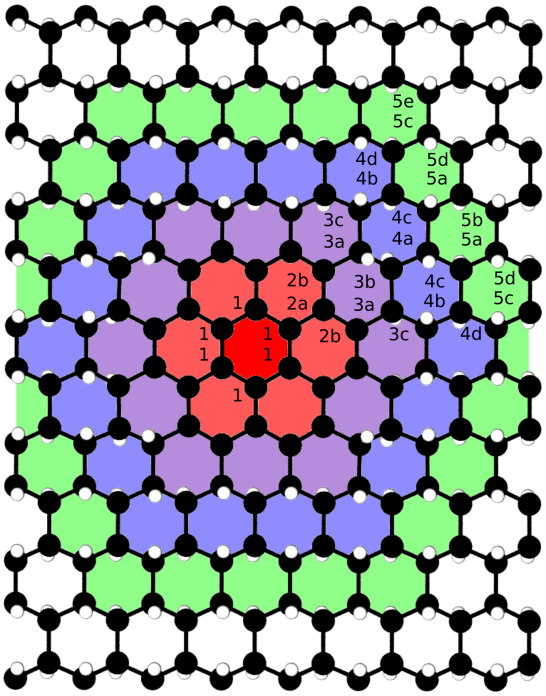

Figure B.1: G2 defected boat-1 supercell. Labeling according to figure 3.7. Defect is colored red.

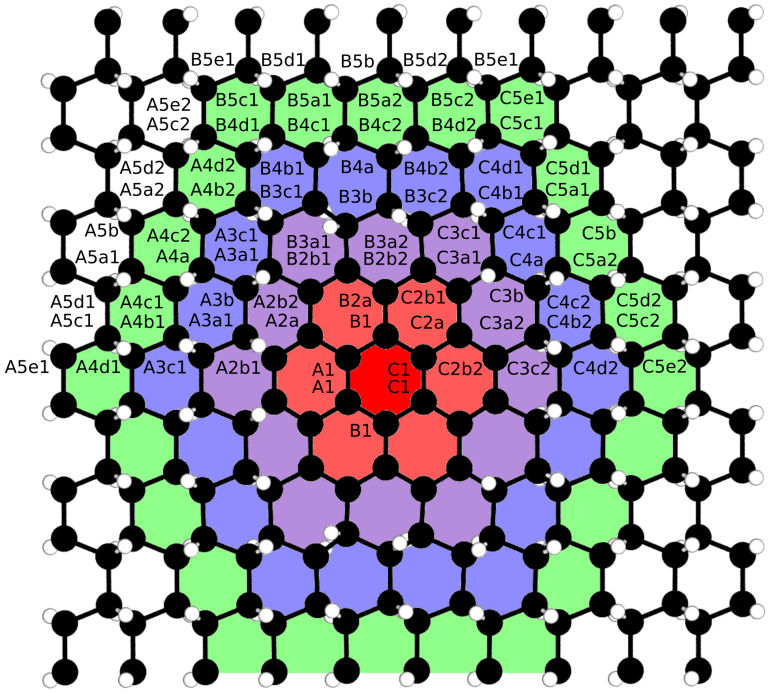

Figure B.2: G2-defected boat-2 supercell. Capital letters in the labeling indicate the closest carbon atom in the defect and the last number of the label tells the side at which the atom is when viewed from defect site: 1 is on the left and 2 on the right.

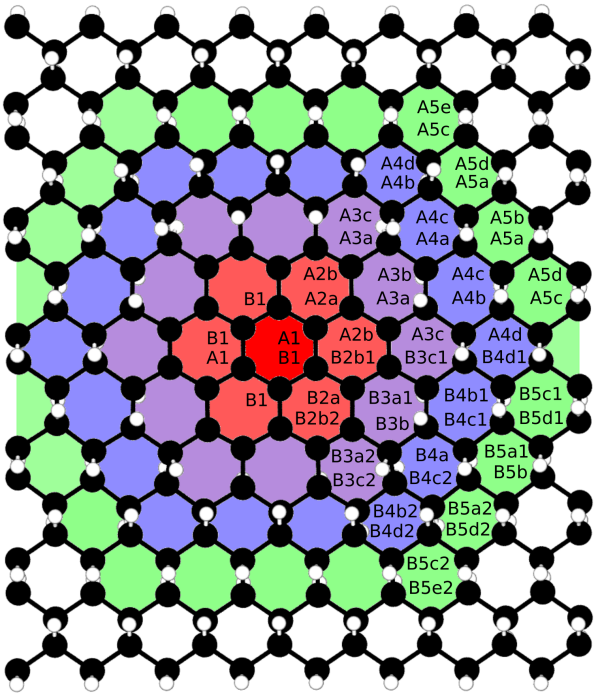

Figure B.3: G2-defected stirrup supercell.

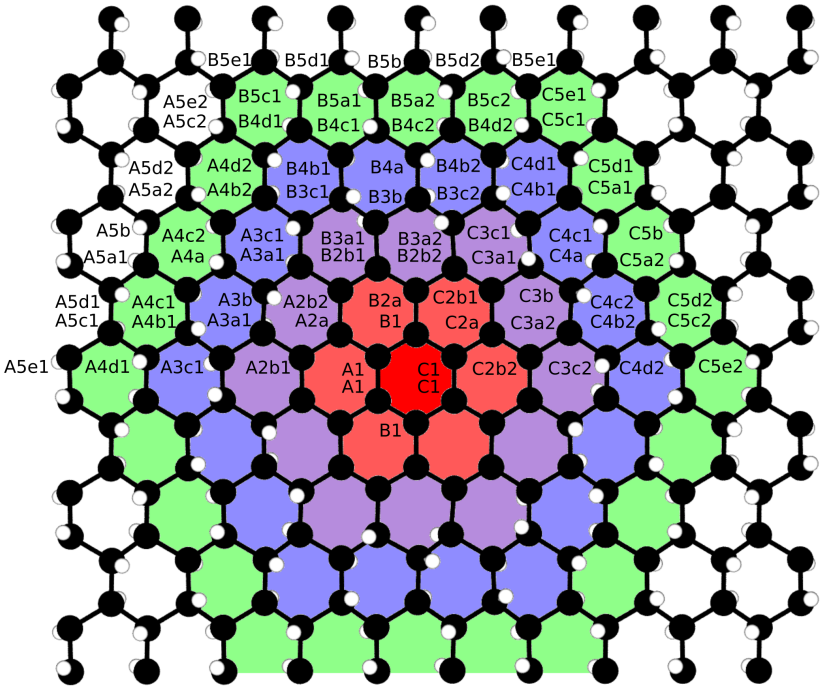

Figure B.4: G2-defected twistboat supercell.

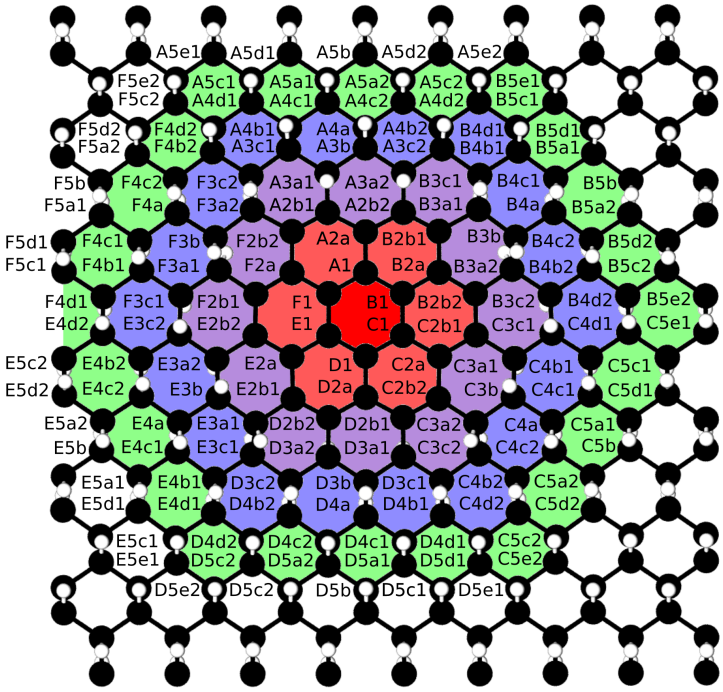

Figure B.5: G2-defected tricycle supercell.

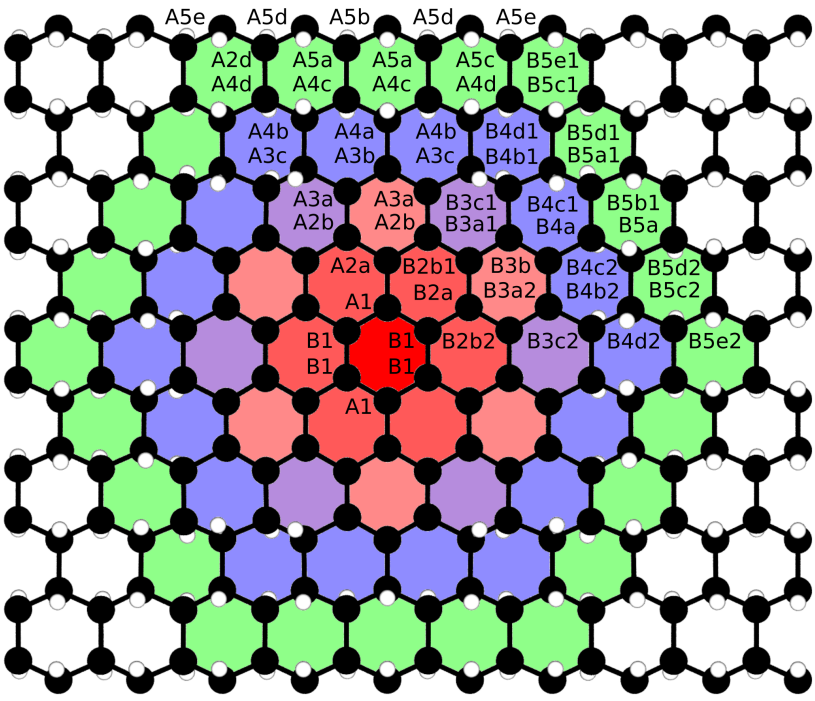

Figure B.6: 2crenG-defected boat-1 supercell.

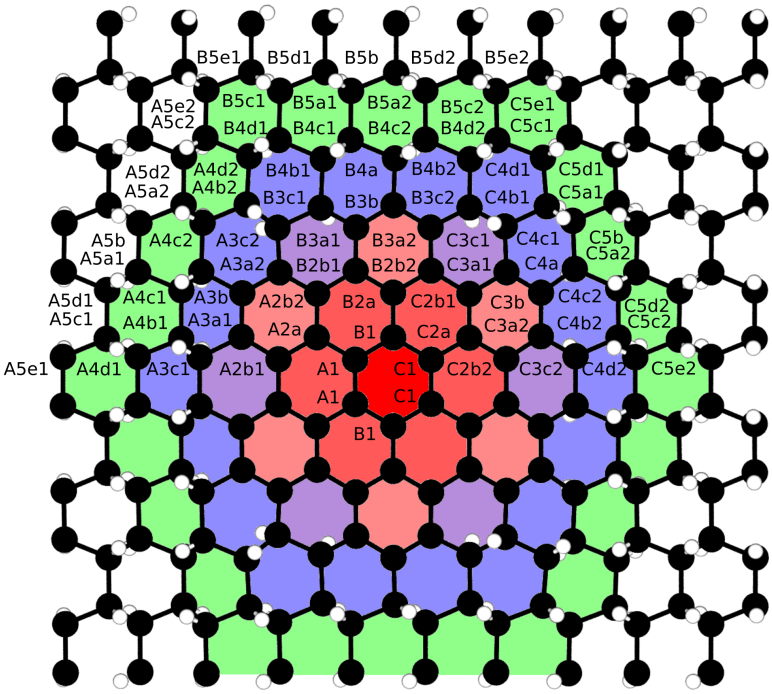

Figure B.7: 2crenG-defected boat-2 supercell.

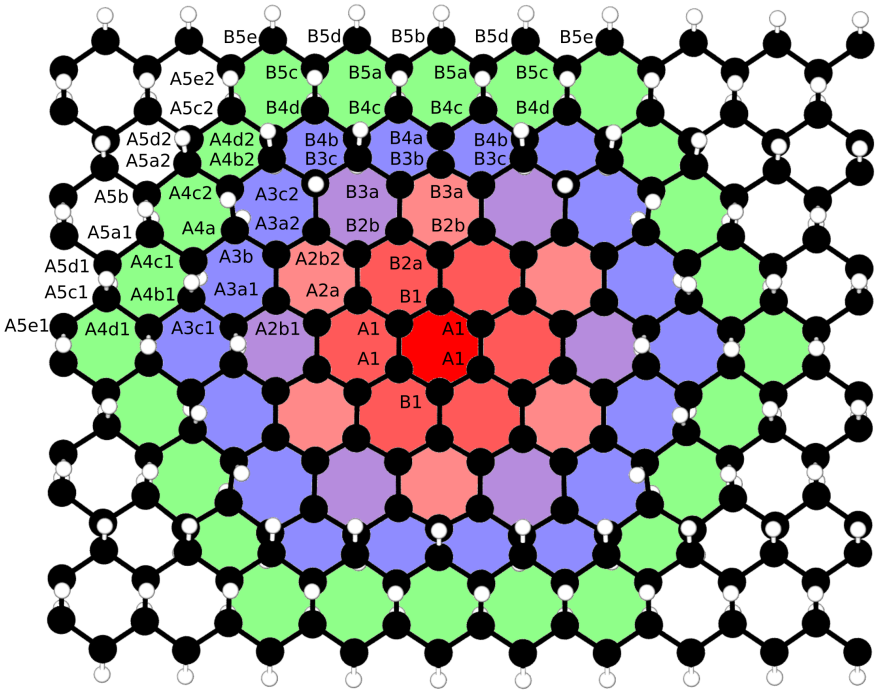

Figure B.8: 2crenG-defected stirrup supercell.

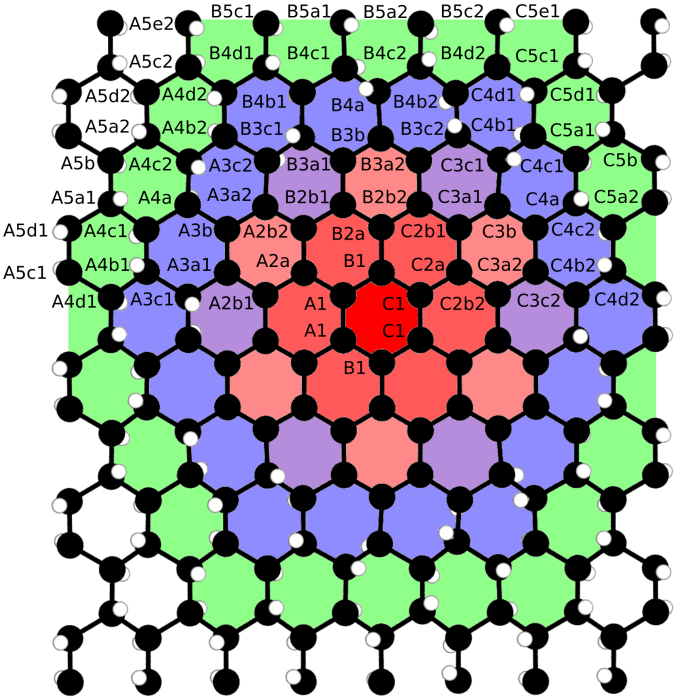

Figure B.9: 2crenG-defected twistboat supercell.

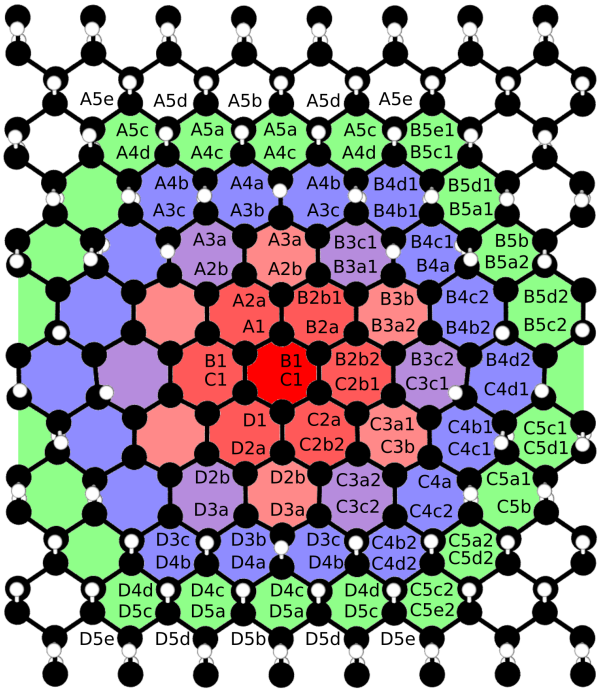

Figure B.10: 2crenG-defected tricycle supercell.

Table B.2: ^{13}C NMR chemical shifts (ppm) in different G2-defected systems.

Conformation	Defect site[a]	Defect side[b]	1	2a	2b	3a	3b	3c	4a	4b	4c	4d	5a	5b	5c	5d	5e
Chair	-	-	141.30	143.47	149.79	67.18	63.37	63.88	72.71	69.32	64.95	65.98	69.58	64.02	64.72	68.48	-
Boat-1	-	-	139.14	143.83	153.32	57.50	52.74	51.16	59.29	56.89	52.93	53.28	54.16	54.47	54.31	55.28	54.15
Boat-2	A	1	139.39	150.73	157.45	56.88	56.99	45.86	45.87	48.29	45.73	45.40	45.16	45.78	45.44	45.51	45.68
		2	-	-	155.71	53.91	-	47.04	-	45.01	46.91	45.40	45.25	-	45.44	45.51	45.71
	B	1	137.11	144.30	151.39	49.10	56.23	56.65	44.67	44.88	49.42	45.71	46.77	47.53	45.84	45.71	45.15
		2	-	-	154.90	51.02	-	48.31	-	46.03	48.61	45.35	46.80	-	46.74	45.97	45.74
	C	1	137.50	142.19	146.90	54.14	47.89	46.92	46.89	46.11	45.52	46.98	45.55	45.45	45.81	44.93	45.45
		2	-	-	152.15	50.90	-	57.30	-	46.13	46.35	46.78	45.17	-	45.85	45.51	45.59
Stirrup	A	-	135.37	142.42	147.52	62.49	48.91	53.77	56.68	56.82	52.19	52.96	53.11	51.94	52.30	53.08	52.76
	B	1	136.14	141.44	148.80	53.04	59.60	59.16	50.87	54.01	55.33	51.97	55.17	55.03	51.88	51.77	53.34
		2	-	-	152.11	53.52	-	50.21	-	52.33	52.24	54.35	53.12	-	52.63	55.14	-
Twistboat	A	1	139.56	144.25	152.08	58.83	63.64	62.83	64.38	67.09	63.19	64.74	64.09	64.59	63.88	65.14	64.40
		2	-	-	155.31	65.90	-	63.41	-	63.07	64.64	64.49	65.12	-	64.83	64.17	64.72
	B	1	139.88	143.77	151.34	63.18	60.60	60.07	69.16	68.32	64.27	65.09	65.38	64.19	64.76	64.30	64.54
		2	-	-	151.70	63.48	-	65.54	-	64.85	63.87	64.87	65.10	-	63.79	64.55	64.88
	C	1	139.83	141.57	154.88	57.55	63.13	64.30	65.18	65.64	63.32	64.72	64.63	64.97	64.34	64.37	64.32
		2	-	-	148.76	65.34	-	64.69	-	62.80	64.91	64.31	64.41	-	64.31	64.24	64.65
Tricycle	A	1	138.35	144.44	145.86	61.46	65.75	64.73	60.23	60.54	59.80	60.20	63.99	64.96	64.76	65.30	65.59
		2	-	-	145.85	61.41	-	64.74	-	60.59	59.70	59.98	63.98	-	64.92	64.96	65.12
	B	1	138.12	142.57	149.36	62.07	63.35	61.13	62.61	65.85	63.35	59.93	65.47	62.95	60.02	65.47	65.60
		2	-	-	148.88	64.09	-	60.38	-	67.04	59.34	64.82	63.11	-	68.55	59.91	65.00
	C	1	137.01	140.30	148.93	59.12	60.13	61.09	67.32	62.80	65.15	62.18	68.25	59.81	62.51	64.94	62.22
		2	-	-	146.75	63.97	-	61.97	-	61.08	59.57	63.18	62.78	-	65.42	63.13	60.10
	D	1	136.15	141.13	146.03	69.33	52.71	61.15	67.98	65.09	64.04	64.70	60.71	59.53	60.30	59.52	60.10
		2	-	-	146.05	69.37	-	61.02	-	65.23	64.02	64.50	63.69	-	60.35	59.49	59.86
	E	1	137.05	140.29	146.79	63.82	59.97	61.93	67.44	60.97	59.33	63.12	62.86	59.63	64.99	62.98	60.35
		2	-	-	148.92	59.08	-	59.08	-	62.82	65.05	62.22	68.44	-	62.34	64.98	-
	F	1	138.18	142.65	149.01	64.01	66.31	60.60	62.53	66.99	59.38	64.78	62.97	63.09	68.34	59.88	-
		2	-	-	149.33	62.10	-	61.21	-	66.05	63.47	59.88	65.62	-	60.23	60.40	65.36

[a] Closest atom in the defect center. [b] The side at which the atom is when viewed from defect site: 1 is on the left and 2 on the right.

Table B.3: ^{1}H NMR chemical shifts (ppm) in different G2-defected systems.

Conformation	Defect site	Defect side	1	2a	2b	3a	3b	3c	4a	4b	4c	4d	5a	5b	5c	5d	5e
Chair	-	-	-	-	-	5.28	3.86	3.64	3.16	3.03	3.08	2.93	2.77	2.83	2.87	2.82	-
Boat-1	-	-	-	-	-	5.01	5.08	4.37	4.32	4.24	4.20	4.05	4.01	3.94	3.97	4.03	3.89
Boat-2	A	1	-	-	-	4.43	4.92	4.95	5.22	5.09	5.35	4.87	4.86	4.93	4.97	5.02	4.92
		2	-	-	-	6.37	-	5.63	-	5.29	5.20	5.16	5.28	-	5.04	5.05	4.98
	B	1	-	-	-	5.72	5.37	5.72	5.31	5.42	5.18	5.18	5.23	5.20	5.23	5.12	5.06
		2	-	-	-	6.10	-	5.15	-	5.39	5.39	5.29	5.23	-	5.16	5.14	5.09
	C	1	-	-	-	6.23	5.71	5.44	4.97	5.31	5.27	5.24	4.91	5.08	4.93	5.14	4.98
		2	-	-	-	6.08	-	4.12	-	4.82	4.98	5.18	5.30	-	4.98	4.96	4.84
Stirrup	A	-	-	-	-	6.40	5.39	5.59	4.06	4.77	4.75	4.91	5.01	4.86	4.84	4.84	4.71
	B	1	-	-	-	6.78	5.04	5.00	5.68	4.75	4.29	5.22	4.48	4.35	5.11	4.88	4.55
		2	-	-	-	5.50	-	5.10	-	4.80	4.95	4.99	5.25	-	5.02	4.70	-
Twistboat	A	1	-	-	-	6.18	5.08	4.31	4.22	4.24	4.33	4.06	3.95	3.93	3.98	3.98	3.92
		2	-	-	-	5.21	-	4.21	-	4.25	4.17	4.05	4.02	-	3.95	3.94	3.91
	B	1	-	-	-	5.64	5.92	4.49	4.44	4.20	4.17	4.08	4.03	3.98	3.96	3.95	3.92
		2	-	-	-	5.92	-	4.33	-	4.30	4.15	4.07	4.04	-	3.99	3.95	3.90
	C	1	-	-	-	5.53	4.72	4.76	4.26	4.19	4.29	4.02	3.99	3.95	3.94	3.89	3.89
		2	-	-	-	5.47	-	5.01	-	4.17	4.11	4.12	4.04	-	3.93	3.92	3.91
Tricycle	A	1	-	-	-	6.07	4.32	4.19	3.56	3.83	3.92	3.67	3.57	3.62	3.67	3.62	3.62
		2	-	-	-	6.08	-	4.2	-	4.20	3.93	3.68	3.57	-	3.68	3.62	3.62
	B	1	-	-	-	6.53	4.23	4.47	4.25	4.00	3.91	4.22	3.76	3.68	3.65	3.76	3.69
		2	-	-	-	5.76	-	4.66	-	4.39	3.34	4.18	3.76	-	4.16	3.24	4.10
	C	1	-	-	-	5.15	4.77	3.73	4.46	3.43	4.29	3.34	4.16	3.19	3.27	4.06	3.30
		2	-	-	-	5.77	-	5.16	-	4.09	3.32	3.79	3.79	-	3.68	3.66	3.77
	D	1	-	-	-	4.97	5.16	5.16	3.8	4.00	3.86	3.82	3.86	3.75	3.82	3.70	3.58
		2	-	-	-	4.98	-	5.16	-	3.99	3.85	3.82	3.85	-	4.00	3.70	3.59
	E	1	-	-	-	5.79	4.77	3.94	4.46	4.11	3.32	3.82	3.81	3.19	3.71	3.71	3.78
		2	-	-	-	5.15	-	3.73	-	3.42	4.26	3.42	4.14	-	4.06	4.14	3.27
	F	1	-	-	-	5.76	4.24	4.67	4.24	4.40	3.34	3.35	3.76	3.67	4.16	3.25	-
		2	-	-	-	6.62	-	4.44	-	3.98	3.89	4.21	3.74	-	3.63	3.74	3.68

Table B.4: ^{13}C NMR chemical shifts (ppm) in different 2crenG-defected systems.

Conformation	Defect site	Defect side	1	2a	2b	3a	3b	3c	4a	4b	4c	4d	5a	5b	5c	5d	5e
Chair	-	-	141.89	143.99	145.75	150.28	150.68	62.78	68.92	67.61	62.06	67.13	71.91	63.21	68.64	63.69	66.38
Boat-1	A	-	141.12	143.02	146.67	151.66	159.24	58.73	55.05	52.50	61.95	56.84	56.03	55.17	55.81	53.34	53.70
	B	1	141.59	142.57	144.87	154.62	155.86	52.38	57.67	61.24	51.85	53.74	57.31	52.67	53.63	55.16	54.35
		2	-	-	144.06	154.75	-	57.54	-	51.92	52.35	56.62	56.58	-	52.98	52.85	55.14
Boat-2	A	1	141.76	140.51	141.60	151.60	157.86	50.36	50.89	54.31	54.70	45.45	45.12	46.27	46.00	45.85	45.61
		2	-	-	141.85	152.15	-	50.65	-	57.58	47.23	45.15	45.19	-	45.70	45.29	46.21
	B	1	141.27	142.31	146.97	148.16	157.02	56.02	50.92	46.97	50.19	48.52	46.60	48.86	47.45	47.44	45.54
		2	-	-	142.65	155.91	-	57.29	-	47.30	53.04	48.65	45.45	-	45.63	47.13	46.19
	C	1	139.84	139.79	146.31	155.40	151.42	55.22	53.39	48.25	48.08	46.74	45.11	45.71	44.17	47.13	45.50
		2	-	-	144.48	150.02	-	53.73	-	47.11	48.23	47.73	47.37	-	45.97	45.36	45.20
Stirrup	A	1	138.65	139.45	144.42	152.32	152.64	56.44	51.82	51.51	51.69	51.42	50.40	54.91	54.36	52.22	54.34
		2	-	-	143.86	146.06	-	56.20	-	50.85	59.18	56.40	53.66	-	53.76	52.34	53.18
	B	-	141.01	144.87	148.16	162.18	156.77	52.97	73.39	60.01	50.85	51.63	56.83	53.01	52.92	52.78	52.36
Twistboat	A	1	141.20	142.88	146.74	151.97	155.10	54.84	57.40	62.51	63.22	65.67	67.94	62.60	65.08	65.08	-
		2	-	-	146.61	152.18	-	64.47	-	63.44	63.64	64.51	65.88	-	65.26	64.80	63.66
	B	1	142.11	143.44	146.14	155.37	156.36	57.28	63.14	67.87	58.12	61.79	67.58	64.85	66.08	64.84	64.91
		2	-	-	144.23	156.00	-	58.63	-	65.75	65.63	64.50	64.81	-	65.37	64.40	63.59
	C	1	141.55	143.18	144.62	152.23	155.04	62.33	65.21	59.83	63.95	66.75	62.18	64.54	64.93	65.02	64.62
		2	-	-	145.13	151.18	-	64.32	-	62.01	63.20	62.71	62.81	-	-	-	-
Tricycle	A	-	140.60	144.45	144.78	150.53	150.26	57.03	61.31	62.86	64.22	65.43	61.36	58.90	60.20	59.80	59.39
	B	1	141.16	142.48	144.96	149.37	151.28	65.68	65.88	63.74	63.24	63.82	61.21	59.48	64.01	62.47	60.55
		2	-	-	145.37	153.81	-	65.44	-	59.61	59.09	63.69	67.90	-	61.90	63.80	-
	C	1	140.37	143.11	146.97	153.16	152.33	61.24	60.48	64.90	59.32	65.19	64.54	62.59	68.59	59.72	-
		2	-	-	146.11	147.01	-	54.93	-	62.87	60.42	59.91	66.31	-	60.83	59.62	64.78
	D	-	143.04	146.33	148.83	159.82	157.91	63.72	76.37	65.21	57.19	58.54	65.70	63.56	64.73	63.99	64.59

Table B.5: ^{1}H NMR chemical shifts (ppm) in different 2crenG-defected systems.

Conformation	Defect site	Defect side	1	2a	2b	3a	3b	3c	4a	4b	4c	4d	5a	5b	5c	5d	5e
Chair	-	-	-	-	-	-	-	5.30	5.10	3.65	3.40	2.96	2.85	2.82	2.76	2.76	2.67
Boat-1	A	-	-	-	-	-	-	5.76	4.95	4.60	3.97	4.28	4.37	4.40	4.19	4.35	4.19
	B	1	-	-	-	-	-	5.50	4.94	4.06	4.58	4.25	4.02	4.00	4.18	3.93	4.04
		2	-	-	-	-	-	5.81	-	4.51	4.17	4.27	4.15	-	3.99	3.92	3.99
Boat-2	A	1	-	-	-	-	-	6.33	5.43	4.55	4.30	4.97	4.86	5.09	5.21	5.04	4.83
		2	-	-	-	-	-	6.02	-	5.11	5.29	5.39	5.26	-	5.09	5.16	5.19
	B	1	-	-	-	-	-	6.40	6.03	5.32	5.10	5.35	5.45	5.47	5.38	5.35	5.28
		2	-	-	-	-	-	5.60	-	5.08	5.44	5.57	5.46	-	5.32	5.24	5.23
	C	1	-	-	-	-	-	6.32	5.50	5.13	5.24	5.51	5.08	5.34	5.25	5.20	5.19
		2	-	-	-	-	-	6.23	-	5.46	5.12	4.77	5.12	-	4.85	4.80	5.10
Stirrup	A	1	-	-	-	-	-	6.26	6.15	4.36	5.08	4.93	5.38	4.24	4.55	4.99	4.83
		2	-	-	-	-	-	6.46	-	5.68	4.74	4.43	4.81	-	4.84	4.97	4.95
	B	-	-	-	-	-	-	7.06	4.65	3.99	4.80	4.76	5.06	5.00	5.24	5.07	4.94
Twistboat	A	1	-	-	-	-	-	6.33	5.50	4.27	4.54	4.58	4.30	4.35	4.36	4.30	4.31
		2	-	-	-	-	-	6.02	-	4.25	4.66	4.37	4.24	-	4.15	4.14	4.07
	B	1	-	-	-	-	-	5.16	5.40	4.18	4.38	4.18	4.22	4.14	4.12	4.19	4.08
		2	-	-	-	-	-	6.18	-	4.65	4.40	4.25	4.34	-	4.14	4.19	4.05
	C	1	-	-	-	-	-	6.08	4.98	4.46	4.12	4.39	4.29	4.20	4.04	4.29	4.17
		2	-	-	-	-	-	5.44	-	4.96	4.75	4.31	4.24	-	-	-	-
Tricycle	A	-	-	-	-	-	-	6.74	6.11	4.63	4.04	3.99	3.93	3.63	4.27	3.70	3.60
	B	1	-	-	-	-	-	5.53	5.88	5.26	3.76	4.07	4.20	3.18	3.79	3.77	4.02
		2	-	-	-	-	-	5.21	-	3.73	4.61	3.39	4.60	-	3.40	4.49	-
	C	1	-	-	-	-	-	5.74	5.69	4.88	3.87	4.83	4.11	4.02	4.72	3.41	-
		2	-	-	-	-	-	6.46	-	4.34	4.44	3.41	4.04	-	3.77	4.05	3.70
	D	-	-	-	-	-	-	6.23	3.69	2.92	4.62	3.87	3.19	3.73	3.50	3.53	3.60

C. Geometries of the investigated systems

Geometries of the investigated systems are presented as xyz-files with addition of the unit cell matrices. All values are in Å.

```
4
pure_1-layer_chair.xyz
C  0.727988695  1.260913407  7.730506998
C  1.455977389  -0.000000000  7.269488551
H  0.727988695  1.260913407  8.840103960
H  1.455977389  -0.000000000  6.159900490

CELL_PARAMETERS (angstrom)
2.183966084  -1.260913407  0.000000000
-0.000000000  2.521826812  0.000000000
0.000000000  0.000000000  20.000000000

8
pure_1-layer_boat1.xyz
C  1.258832747  0.782799334  7.824773603
C  0.000000000  2.929719844  7.175337992
C  1.258832747  3.510685220  7.824773603
C -0.000000000  1.363764709  7.175337992
H  1.258832747  1.101647697  8.882317241
H  0.000000000  3.248252674  6.117571165
H  1.258832747  3.191836857  8.882317241
H  0.000000000  1.045231880  6.117571165

CELL_PARAMETERS (angstrom)
2.517665494  0.000000000  0.000000000
0.000000000  4.293484554  0.000000000
0.000000000  0.000000000  20.000000000

16
pure_1-layer_boat2.xyz
C  6.926093988  2.681909854  1.856181180
C  8.073867734  1.842951422  4.004348911
C  8.073867734  0.419476880  1.856185819
C  8.073867734  1.842951422  2.440140366
C  6.926093988  4.105375052  4.004344272
C  6.926093988  2.681909854  0.291981913
C  6.926093988  4.105375052  2.440145005
C  8.073867734  0.419476880  0.291977273
H  5.982355817  2.210435119  2.171840290
H  9.017682461  2.314358041  0.023643535
H  9.017682461  4.472926864  2.171806627
H  9.017682461  2.314358041  2.124519558
H  5.982355817  0.051993182  0.023677198
H  5.982355817  2.210435119  4.272648987
H  5.982355817  0.051993182  2.124485895
H  9.017682461  4.472926864  4.272682650

CELL_PARAMETERS (angstrom)
20.000000000  0.000000000  0.000000000
0.000000000  4.524856603  0.000000000
0.000000000  0.000000000  4.296326185

8
pure_1-layer_stirrup.xyz
C  0.000000000  5.570967891  1.387312150
C  1.268733137  4.429037637  3.292123084
C -0.000000000  4.429037637  2.422367451
C  1.268733137  5.570967891  0.517518028
H -0.000000000  6.525817208  1.943073289
H  1.268733137  3.474177264  3.847891353
H -0.000000000  3.474177264  1.866599182
H  1.268733137  6.525817208  -0.038243111

CELL_PARAMETERS (angstrom)
2.537466275  0.000000000  0.000000000
0.000000000  20.000000000  0.000000000
0.000000000  0.000000000  3.809660357

16
pure_1-layer_twistboat.xyz
C  0.395371267  7.185872191  3.129664320
C  3.921430437  7.185872191  4.470129780
C  1.763029585  7.185872191  0.596399620
C  3.921800542  7.814049680  1.936703119
C  1.763399690  7.814049680  3.129826281
C  0.395001162  7.814049680  0.596561581
C  2.553402014  7.814049680  4.469967819
C  2.553772119  7.185872191  1.936865080
H  0.525135007  6.127146707  2.844050447
H  3.791666697  6.127146707  4.755743653
H  1.633265845  6.127146707  0.310785747
H  3.792072860  8.872931422  2.222341780
H  1.633672008  8.872931422  2.844187619
H  0.524728844  8.872931422  0.310922920
H  2.683129696  8.872931422  4.755606480
H  2.683535859  6.127146707  2.222478953

CELL_PARAMETERS (angstrom)
4.316801704  0.000000000  0.000000000
0.000000000  20.000000000  0.000000000
0.000000000  0.000000000  5.066529400

16
pure_1-layer_tricycle.xyz
C  7.480718692  0.430880620  0.633443356
C  7.519233895  7.143190010  1.900330069
C  7.519233895  4.217763345  0.633443356
C  7.480718692  3.356103831  1.900330069
C  8.622683917  1.460250924  0.633443356
C  6.377395221  6.113719099  1.900330069
C  6.377395221  5.247234256  0.633443356
C  8.622683917  2.326733528  1.900330069
H  6.511787034  0.966756356  0.633443356
H  8.488179338  6.607342638  1.900330069
H  8.488179338  4.753610716  0.633443356
H  6.511787034  2.820228096  1.900330069
H  9.565352582  0.876634151  0.633443356
H  5.434649321  6.697221759  1.900330069
H  5.434649321  4.663731595  0.633443356
H  9.565352582  2.910350301  1.900330069

CELL_PARAMETERS (angstrom)
20.000000000  0.000000000  0.000000000
0.000000000  7.573968903  0.000000000
0.000000000  0.000000000  2.533773426

8
pure_2-layer_chair_aa.xyz
C  0.728415028  1.263738048  7.669989451
C  1.456729875  0.005516145  7.209229273
H  0.728322190  1.263963392  8.779685559
H  1.456822219  0.005290866  6.099586593
C  0.728480880  1.263496974  1.792542556
C  1.456795679  0.005275173  1.331766700
H  0.728388215  1.263721269  2.902189868
H  1.456887724  0.005050545  0.222078765

CELL_PARAMETERS (angstrom)
2.184936987  -1.252011825  0.000000000
0.000377092  2.521014146  0.000000000
0.000000000  0.000000000  24.350000000

8
pure_2-layer_chair_ab.xyz
C  1.252143  0.722924  6.662561
C  -0.000001  1.445850  7.121653
H  1.252143  0.722924  5.552305
H  -0.000001  1.445850  8.231909
C  2.504284  0.000000  11.561810
C  1.252143  0.722924  12.020851
H  2.504284  0.000000  10.451680
H  1.252143  0.722924  13.130981

CELL_PARAMETERS (angstrom)
2.504284  0.000000  0.000000
-1.252142  2.168773  0.000000
0.000000  0.000000  24.402765

16
pure_2-layer_boat1_ab.xyz
C  1.254302555  0.918361018  7.857634380
C  0.000000000  3.059210815  7.208832590
C  1.254302555  3.637569081  7.860793537
C  0.000000000  1.497500497  7.206963490
H  1.254302555  1.240067772  8.913333168
H  0.000000000  3.381646973  6.152810523
H  1.254302555  3.320022792  8.916588941
H  0.000000000  1.176767704  6.150439694
C  1.254302555  2.002467446  12.082664304
C  0.000000000  4.142243113  11.429680586
C  1.254302555  4.720779112  12.081434961
C  0.000000000  2.581560168  11.432045980
H  1.254302555  2.323714632  13.139045482
H  0.000000000  4.460394920  10.373985044
H  1.254302555  4.398873687  13.137566693
H  0.000000000  2.260347576  10.376180626

CELL_PARAMETERS (angstrom)
2.508605111  0.000000000  0.000000000
0.000000000  4.280005245  0.000000000
0.000000000  0.000000000  28.000000000

32
pure_2-layer_boat2_ab.xyz
C  6.854162867  2.646336258  1.606918409
C  8.015374000  1.828394223  3.747039710
C  8.015374000  0.408902539  1.607394387
C  8.014687074  1.828264108  2.187370330
C  6.854162867  4.065554026  3.746563732
C  6.855506503  2.646726099  0.048005487
C  6.855506503  4.065164186  2.187650810
C  8.014687074  0.409032654  0.047725007
H  5.919206923  2.163238835  1.926060968
H  8.950784433  2.310716633  -0.211492712
H  8.950784433  4.401173652  1.928152612
H  8.949558135  2.311213761  1.866207591
H  5.919206923  0.074057927  -0.213584356
H  5.921983107  2.161031528  4.006163138
H  5.921983107  0.076265233  1.866517814
H  8.949558135  4.400676525  4.005852914
C  2.004777693  2.646187227  0.536952265
C  3.164027822  1.828015849  2.676266980
C  3.164027822  0.409280912  0.536621656
C  3.165252471  1.828075056  1.117426894
C  2.004777693  4.065703058  2.676597588
C  2.004254465  2.646369903  -1.022600753
C  2.004254465  4.065520381  1.117044571
C  3.165252471  0.409221706  -1.022218429
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H  1.069817925  2.163159221  0.857799968
H  4.097649501  2.313675225  -1.282125417
H  4.097649501  4.398215061  0.857519907
H  4.100064190  2.311065617  0.797787946
H  1.069817925  0.074137540  -1.281845355
H  1.068892892  2.164031070  2.935790605
H  1.068892892  0.073265691  0.796145281
H  4.100064190  4.400824669  2.937433270

CELL_PARAMETERS (angstrom)
31.000000000  0.000000000  0.000000000
0.000000000  4.474593523  0.000000000
0.000000000  0.000000000  4.279290648

16
pure_2-layer_stirrup_ab.xyz
C  0.000000000  2.967534471  1.322800865
C  1.263749428  1.809343980  3.199943016
C  0.000000000  1.809462426  2.333105287
C  1.263749428  2.968885843  0.455895275
H  0.000000000  3.911393351  1.895013021
H  1.263749428  0.866346604  3.772884229
H  0.000000000  0.866237866  1.760333635
H  1.263749428  3.912981753  -0.113602991
C  0.000000000  7.730703875  2.767525759
C  1.263749428  6.570879294  4.644685042
C  0.000000000  6.572091305  3.777795386
C  1.263749428  7.730484949  1.900637861
H  0.000000000  8.674120980  3.340234366
H  1.263749428  5.627081001  5.214746663
H  0.000000000  5.628673078  3.205025142
H  1.263749428  8.673779224  1.327784067

CELL_PARAMETERS (angstrom)
2.527498857  0.000000000  0.000000000
0.000000000  31.000000000  0.000000000
0.000000000  0.000000000  3.753632373

32
pure_2-layer_twistboat_ab.xyz
C  0.025555365  2.128701084  3.116925908
C  3.543310486  2.129479035  4.453396034
C  1.389681029  2.129479035  0.593385728
C  3.542685700  2.760213458  1.929223251
C  1.389056243  2.760213458  3.117558512
C  0.026112606  2.761029075  0.594333224
C  2.179742063  2.761029075  4.452448538
C  2.179184822  2.128701084  1.929855854
H  0.153545287  1.071172620  2.826683460
H  3.415649016  1.072167976  4.744385951
H  1.262019559  1.072167976  0.302395811
H  3.410658540  3.816851491  2.217708748
H  1.257029083  3.816851491  2.829073014
H  0.157695646  3.818107559  0.306681566
H  2.311325103  3.818107559  4.740100196
H  2.307174744  1.071172620  2.220098302
C  2.139262395  6.739997483  3.117333727
C  5.655664857  6.738749295  4.452212667
C  3.502035399  6.738749295  0.594569096
C  5.656260066  7.371720912  1.929643802
C  3.502630609  7.371720912  3.117137960
C  2.138416292  7.370378840  0.593262352
C  4.292045749  7.370378840  4.453519410
C  4.292891852  6.739997483  1.929448035
H  2.271862875  5.683398368  2.828580334
H  5.524730013  5.681451236  4.739596945
H  3.371100556  5.681451236  0.307184817
H  5.528900754  8.429118400  2.220188507
H  3.375271297  8.429118400  2.826593255
H  2.266777781  8.427463166  0.301984958
H  4.420407238  8.427463166  4.744796804
H  4.425492332  5.683398368  2.218201428

CELL_PARAMETERS (angstrom)
4.307258914  0.000000000  0.000000000
0.000000000  30.000000000  0.000000000
0.000000000  0.000000000  5.046781762

32
pure_2-layer_tricycle_ab.xyz
C  2.999201973  0.911561796  0.631026047
C  3.021112797  7.492578661  1.893078142
C  3.018544989  4.633861505  0.631026047
C  2.997131263  3.774284722  1.893078142
C  4.161107902  1.911849030  0.631026047
C  1.855318652  6.496323792  1.893078142
C  1.854522259  5.631552088  0.631026047
C  4.160851489  2.776382573  1.893078142
H  2.043242701  1.468256171  0.631026047
H  3.973781707  6.931663652  1.893078142
H  3.971966552  5.193412543  0.631026047
H  2.042356656  3.215543089  1.893078142
H  5.090172181  1.310872232  0.631026047
H  0.926983919  7.101062963  1.893078142
H  0.925338164  5.028122887  0.631026047
H  5.089673488  3.379738928  1.893078142
C  8.180717404  1.037379430  0.631026047
C  8.202972865  7.618361338  1.893078142
C  8.200882089  4.755859024  0.631026047
C  8.179554121  3.896515005  1.893078142
C  9.345174899  2.035176778  0.631026047
C  7.039893989  6.619376295  1.893078142
C  7.038492145  5.754857503  0.631026047
C  9.345035302  2.900207104  1.893078142
H  7.227233964  1.596876267  0.631026047
H  9.158400611  7.060767420  1.893078142
H  9.155938548  5.314045105  0.631026047
H  7.226809261  3.335687526  1.893078142
H 10.273847137  1.430944252  0.631026047
H  6.111582146  7.221591463  1.893078142
H  6.108829915  5.152754992  0.631026047
H 10.273328916  3.504832258  1.893078142

CELL_PARAMETERS (angstrom)
31.000000000  0.000000000  0.000000000
0.000000000  7.440930502  0.000000000
0.000000000  0.000000000  2.524104189

12
pure_3-layer_chair_aa.xyz
H  -0.000001  1.445849  17.850973
C  -0.000001  1.445849  16.740834
C  1.252143  0.722923  16.281809
H  1.252143  0.722923  15.171670
H  -0.000001  1.445849  13.130973
C  -0.000001  1.445849  12.020834
C  1.252143  0.722923  11.561809
H  1.252143  0.722923  10.451670
H  -0.000001  1.445849  8.410973
C  -0.000001  1.445849  7.300834
C  1.252143  0.722923  6.841809
H  1.252143  0.722923  5.731670

CELL_PARAMETERS (angstrom)
2.504284  0.000000  0.000000
-1.252142  2.168773  0.000000
0.000000  0.000000  28.403218

12
pure_3-layer_chair_ab.xyz
H -0.000001  1.445849  17.850973
C -0.000001  1.445849  16.740834
C  1.252143  0.722923  16.281809
H  1.252143  0.722923  15.171670
H  1.252143  0.722923  13.130973
C  1.252143  0.722923  12.020834
C  2.504283  0.000000  11.561809
H  2.504283  0.000000  10.451670
H  -0.000001  1.445849  8.410973
C  -0.000001  1.445849  7.300834
C  1.252143  0.722923  6.841809
H  1.252143  0.722923  5.731670

CELL_PARAMETERS (angstrom)
2.504284  0.000000  0.000000
-1.252142  2.168773  0.000000
0.000000  0.000000  28.403218

24
pure_3-layer_boat1_ab.xyz
C  1.254185495  0.872248000  7.887353989
C  0.000000000  3.012718988  7.237355702
C  1.254185495  3.591080819  7.889180824
C  0.000000000  1.451245984  7.236647319
H  1.254185495  1.193168335  8.943269304
H  0.000000000  3.334382152  6.181152016
H  1.254185495  3.271882166  8.944589235
H  0.000000000  1.129831587  6.180357111
C  1.254185495  1.941837337  12.115812947
C  0.000000000  4.081370102  11.462719069
C  1.254185495  4.661163642  12.113121325
C  0.000000000  2.521503773  11.465439448
H  1.254185495  2.260365288  13.171671478
H  0.000000000  4.399567571  10.406799616
H  1.254185495  4.340762847  13.169363197
H  0.000000000  2.200800690  10.409273034
C  1.254185495  0.886779880  16.343372296
C  0.000000000  3.025487580  15.693451269
C  1.254185495  3.604496415  16.344089900
C  0.000000000  1.465081981  15.691523838
H  1.254185495  1.208584988  17.399534722
H  0.000000000  3.346088994  14.637425438
H  1.254185495  3.283241656  17.400437579
H  0.000000000  1.145827683  14.636059343

CELL_PARAMETERS (angstrom)
2.508370991  0.000000000  0.000000000
0.000000000  4.279178021  0.000000000
0.000000000  0.000000000  32.000000000

48
pure_3-layer_boat2_ab.xyz
C  7.815237942  2.645363111  1.528935141
C  8.976538342  1.827415412  3.668015233
C  8.976538342  0.408980406  1.528751480
C  8.974814435  1.827391028  2.109480182
C  7.815237942  4.063824344  3.668198894
C  7.816940480  2.645439632  -0.029598909
C  7.816940480  4.063747824  2.109664844
C  8.974814435  0.409004791  -0.029783571
H  6.880150812  2.162860988  1.848597517
H  9.911893678  2.309674425  -0.291203231
H  9.911893678  4.399513031  1.848060523
H  9.908569933  2.312779000  1.788384819
H  6.880150812  0.073534831  -0.290666236
H  6.883199912  2.160015262  3.928202603
H  6.883199912  0.076380555  1.788938850
H  9.908569933  4.396408456  3.927648572
C  2.970180196  2.644764223  0.461565615
C  4.129749023  1.827549700  2.600371374
C  4.129749023  0.408846119  0.461107621
C  4.130931591  1.827377866  1.041806325
C  2.970180196  4.064423233  2.600829368
C  2.969744084  2.645273798  -1.097598281
C  2.969744084  4.063913658  1.041665473
C  4.130931591  0.409017953  -1.097457429
H  2.035436411  2.161485350  0.782762468
H  5.063279456  2.313356680  -1.357429482
H  5.063279456  4.395830776  0.781834272
H  5.065349731  2.310494154  0.721610536
H  2.035436411  0.074910468  -1.356501285
H  2.034357340  2.163152363  2.859869162
H  2.034357340  0.073243454  0.720605409
H  5.065349731  4.398693302  2.860874289
C 12.674344530  2.645502550  0.447142218
C 13.834085351  1.827657700  2.586751071
C 13.834085351  0.408738119  0.447487318
C 13.834621280  1.827806584  1.027405734
C 12.674344530  4.063684905  2.586405971
C 12.673389863  2.644975070  -1.111578074
C 12.673389863  4.064212387  1.027685680
C 13.834621280  0.408589235  -1.111858019
H 11.740445144  2.160348566  0.768291677
H 14.768694243  2.310943348  -1.370419603
H 14.768694243  4.398244108  0.768844151
H 14.769726342  2.310489426  0.706430609
H 11.740445144  0.076047252  -1.370972076
H 11.738319882  2.162171391  2.847465038
H 11.738319882  0.074224428  0.708201285
H 14.769726342  4.398698030  2.845694364

CELL_PARAMETERS (angstrom)
37.000000000  0.000000000  0.000000000
0.000000000  4.472791637  0.000000000
0.000000000  0.000000000  4.278527506

24
pure_3-layer_stirrup_ab.xyz
C  0.000000000  3.756045771  1.329322701
C  1.263531417  2.597696041  3.206161091
C  0.000000000  2.597607959  2.339196398
C  1.263531417  3.757044950  0.462645574
H  0.000000000  4.699234212  1.902117150
H  1.263531417  1.654163895  3.778399699
H  0.000000000  1.654343053  1.766399101
H  1.263531417  4.700257498  -0.107722254
C  0.000000000  8.496025082  2.787059213
C  1.263531417  7.337030265  4.663123594
```

```
C  0.000000000  7.338312091  3.796756517
C  1.263531417  8.494887481  1.920529989
H  0.000000000  9.440098303  3.356493365
H  1.263531417  6.393281197  5.232837300
H  0.000000000  6.395268533  3.223568325
H  1.263531417  9.438507184  1.348142843
C  0.000000000  13.245880392  1.344920159
C  1.263531417  12.087260920  3.220940790
C  0.000000000  12.086447922  2.354139868
C  1.263531417  13.245794210  0.478204224
H  0.000000000  14.189275162  1.917468419
H  1.263531417  11.143739766  3.793444530
H  0.000000000  11.142783311  1.784252914
H  1.263531417  14.189014801  -0.094588917

CELL_PARAMETERS (angstrom)
2.527062835  0.000000000  0.000000000
0.000000000  35.000000000  0.000000000
0.000000000  0.000000000  3.752588477

48
pure_3-layer_twistboat_ab.xyz
C  0.135746689  3.093858561  3.117027506
C  3.651570005  3.093789930  4.453427500
C  1.499380464  3.093789930  0.593422456
C  3.650796475  3.725484073  1.929083879
C  1.498606933  3.725484073  3.117766078
C  0.136596965  3.725495232  0.594372240
C  2.288786507  3.725495232  4.452477716
C  2.287936230  3.093858561  1.929822450
H  0.263447490  2.036459197  2.826462660
H  3.523937314  2.036401825  4.744392970
H  1.371747773  2.036401825  0.302456986
H  3.518650539  4.782201549  2.217150201
H  1.366460998  4.782201549  2.829699755
H  0.268885050  4.782235838  0.306336673
H  2.421074591  4.782235838  4.740513283
H  2.415637033  2.036459197  2.220387297
C  2.285540233  7.684352972  3.117476540
C  5.800643543  7.684487540  4.452531698
C  3.648454001  7.684487540  0.594318258
C  5.800647319  8.315550233  1.929111692
C  3.648457777  8.315550233  3.117738264
C  2.285544067  8.315607565  0.594056518
C  4.437733610  8.315607565  4.452793439
C  4.437729774  7.684352972  1.929373416
H  2.416847786  6.627194971  2.829999596
H  5.669435487  6.627324989  4.740127347
H  3.517245945  6.627324989  0.306722609
H  5.669437170  9.372658305  2.216697995
H  3.517247628  9.372658305  2.830151960
H  2.416849541  9.372820202  0.306571007
H  4.569039083  9.372820202  4.740278948
H  4.569037329  6.627194971  2.216850360
C  0.136598696  12.274501589  3.117796779
C  3.650795289  12.274523029  4.452507981
C  1.498605748  12.274523029  0.594341975
C  3.651569758  12.906213905  1.930003088
C  1.499380216  12.906213905  3.116846869
C  0.135749317  12.906135220  0.593603544
C  2.287938859  12.906135220  4.453246412
C  2.288788239  12.274501589  1.929053176
H  0.268885469  11.217766150  2.829761912
H  3.518650781  11.217796209  4.740576228
H  1.366461238  11.217796209  0.306273727
H  3.523938051  13.963597183  2.220967628
H  1.371748509  13.963597183  2.825882329
H  0.263448388  13.963543733  0.303037156
H  2.415637930  13.963543733  4.743812799
H  2.421075011  11.217766150  2.217088043

CELL_PARAMETERS (angstrom)
4.304379083  0.000000000  0.000000000
0.000000000  36.000000000  0.000000000
0.000000000  0.000000000  5.046849955

48
pure_3-layer_tricycle_ab.xyz
C  3.811656177  0.782196281  0.630923281
C  3.833137936  7.362280346  1.892769844
C  3.833948807  4.504464127  0.630923281
C  3.812409080  3.644795893  1.892769844
C  4.974742636  1.780897534  0.630923281
C  2.668192352  6.365465509  1.892769844
C  2.668491342  5.500717245  0.630923281
C  4.974615741  2.645451441  1.892769844
H  2.856677733  1.340555235  0.630923281
H  4.785950060  6.801710836  1.892769844
H  4.786609406  5.065209987  0.630923281
H  2.856901169  3.087250943  1.892769844
H  5.903493557  1.178270840  0.630923281
H  1.739748548  6.969934593  1.892769844
H  1.740304069  4.895776031  0.630923281
H  5.903492241  3.247735630  1.892769844
C  8.993397293  0.765566946  0.630923281
C  9.015299236  7.345413384  1.892769844
C  9.013755004  4.485876504  0.630923281
C  8.992030037  3.626079743  1.892769844
C 10.156147382  1.764360732  0.630923281
C  7.851247547  6.348381369  1.892769844
C  7.850726198  5.484033199  0.630923281
C 10.156002876  2.628834898  1.892769844
H  8.039371387  1.324479068  0.630923281
H  9.968738640  6.785481703  1.892769844
H  9.967656284  5.045022064  0.630923281
H  8.038797957  3.065742481  1.892769844
H 11.084518519  1.161951045  0.630923281
H  6.923374473  6.952433806  1.892769844
H  6.922258915  4.881189890  0.630923281
H 11.084198268  3.232655135  1.892769844
C 14.159920319  0.832319013  0.630923281
C 14.182123846  7.412234172  1.892769844
C 14.187059204  4.549851820  0.630923281
C 14.165347630  3.690205868  1.892769844
C 15.326828787  1.827188618  0.630923281
C 13.021050762  6.411349579  1.892769844
C 13.022490644  5.546886928  0.630923281
C 15.328769498  2.691955483  1.892769844
H 13.207815666  1.393782885  0.630923281
H 15.138338506  6.855925831  1.892769844
H 15.141783788  5.108497649  0.630923281
H 13.211826497  3.130883535  1.892769844
H 16.253919084  1.220553280  0.630923281
H 12.091607946  7.012016425  1.892769844
H 12.094832220  4.942355736  0.630923281
H 16.258394734  3.294787496  1.892769844

CELL_PARAMETERS (angstrom)
38.000000000  0.000000000  0.000000000
0.000000000  7.439839769  0.000000000
0.000000000  0.000000000  2.523693126

8
pure_bulk_chair_aa.xyz
C  0.728822623  1.262357812  5.412862031
C  1.457645245  0.000000000  4.950116946
H  0.728822623  1.262357812  6.518143160
H  1.457645245  0.000000000  3.844869019
C  0.728822623  1.262357812  1.066985569
C  1.457645245  -0.000000000  0.604238069
H  0.728822623  1.262357812  2.172236067
H  1.457645245  -0.000000000  -0.501045040

CELL_PARAMETERS (angstrom)
2.186467868  -1.262357812  0.000000000
0.000000000  2.524715624  0.000000000
0.000000000  -0.000000000  8.691368769

8
pure_bulk_chair_ab.xyz
C  0.728376440  1.261585001  1.515738687
C  1.456752880  -0.000000000  1.053361973
H  0.728376440  1.261585001  2.621660589
H  1.456752880  -0.000000000  -0.053395870
C  1.456752880  -0.000000000  5.960455052
C  0.000000000  2.523170002  5.498125472
H  1.456752880  -0.000000000  7.067155528
H  0.000000000  2.523170002  4.392215195

CELL_PARAMETERS (angstrom)
2.185129320  -1.261585001  -0.000000000
0.000000000  2.523170002  -0.000000000
-0.000000000  -0.000000000  9.313562721

16
pure_bulk_boat1_ab.xyz
C  1.257493575  0.967847587  5.956320830
C  0.000000000  3.104625844  5.293484770
C  1.257493575  3.690876112  5.938948609
C  0.000000000  1.544918625  5.302535508
H  1.257493575  1.294245007  7.007390971
H  0.000000000  3.416254598  4.238046831
H  1.257493575  3.380304008  6.993663932
H  0.000000000  1.219409775  4.252545925
C  1.257493575  2.065620894  10.119173803
C  0.000000000  4.202318015  9.451903082
C  1.257493575  4.788573150  10.097288336
C  0.000000000  2.642536897  9.465382130
H  1.257493575  2.390434785  11.169423453
H  0.000000000  4.512309331  8.397013977
H  1.257493575  4.476295780  11.152484300
H  0.000000000  2.315505836  8.414496084

CELL_PARAMETERS (angstrom)
2.514987150  0.000000000  0.000000000
0.000000000  4.282819144  -0.030117879
0.000000000  0.058017045  8.327522159

32
pure_bulk_boat2_ab.xyz
C  5.609719437  2.650431726  1.600948567
C  6.771439660  1.829198235  3.741572911
C  6.770083103  0.410610022  1.600191225
C  6.769080827  1.829222531  2.182245959
C  5.611075994  4.068993046  3.742330252
C  5.610149185  2.650382529  0.041622147
C  5.611505743  4.069042243  2.183003832
C  6.767724270  0.410585726  0.040864273
H  4.676203036  2.168778528  1.920655304
H  7.702536089  2.310973973  -0.222660500
H  7.703892646  4.408450799  1.918721185
H  7.701524549  2.313461259  1.861715522
H  4.674846479  0.071029729  -0.220726381
H  4.680141924  2.165968220  4.005055360
H  4.678785367  0.073840037  1.863673675
H  7.702881106  4.405963513  4.003097207
C  0.740213908  2.650432069  0.539543712
C  1.899096386  1.829239244  2.680249835
C  1.897739828  0.410569013  0.538868149
C  1.899411611  1.829138059  1.120931695
C  0.741570465  4.068992702  2.680925398
C  0.737879378  2.650413450  -1.019779494
C  0.739235935  4.069011322  1.121602191
C  1.898055054  0.410670198  -1.020449990
H -0.192241488  2.166316034  0.860033344
H  2.829113521  2.313636162  -1.283173652
H  2.830470078  4.405788610  0.858208033
H  2.832815520  2.310808443  0.801190280
H -0.193598045  0.073492224  -1.281348342
H -0.193156065  2.168558507  2.944390327
H -0.194512622  0.071249750  0.803008642
H  2.834172077  4.408616329  2.942571966

CELL_PARAMETERS (angstrom)
9.740773388  0.000000000  -0.005954735
0.000000000  4.479616514  0.000000000
0.002713114  0.000000000  4.282763371

16
pure_bulk_stirrup_ab.xyz
C  0.000000000  1.691342449  1.335381186
C  1.264275887  0.529525829  3.209711690
C  0.000000000  0.529513400  2.343388042
C  1.264275887  1.694115531  0.469258656
H  0.000000000  2.631183055  1.910316934
H  1.264275887  -0.412119403  3.781505548
H  0.000000000  -0.410838265  1.771513886
H  1.264275887  2.636275728  -0.099512472
C  0.000000000  6.455273741  2.776495105
C  1.264275887  5.290677820  4.650716552
C  0.000000000  5.293660318  3.784803850
C  1.264275887  6.455240266  1.910434891
H  0.000000000  7.395781585  3.347965685
H  1.264275887  4.348270025  5.219211249
H  0.000000000  4.353975996  3.209669504
H  1.264275887  7.396974922  1.338543736

CELL_PARAMETERS (angstrom)
2.528551773  0.000000000  0.000000000
0.000000000  9.529717785  0.028789892
0.000000000  -0.006248046  3.752305749

32
pure_bulk_twistboat_ab.xyz
C  0.377697676  0.622681432  3.121625332
C  3.897097015  0.764671792  4.458601825
C  1.742982581  0.679987930  0.593797538
C  3.871244615  1.392268271  1.931737357
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C  1.717130181  1.307584409  3.120662006
C  0.353630818  1.257558139  0.595832454
C  2.507745252  1.342242000  4.456566909
C  2.531812109  0.707365294  1.930774031
H  0.547125788 -0.427599901  2.836825254
H  3.809857292 -0.293867798  4.748150522
H  1.655742858 -0.378551660  0.304248841
H  3.696561458  2.440755326  2.218340284
H  1.542447024  2.356071464  2.834059079
H  0.442971726  2.317594301  0.312873137
H  2.597086160  2.402278163  4.739526226
H  2.701240222 -0.342916039  2.215574109
C  2.303521730  5.357772456  3.120647839
C  5.821290211  5.492192401  4.456421475
C  3.667175778  5.407508540  0.595977888
C  5.797203944  6.127328563  1.930645431
C  3.643089510  6.042644701  3.121753932
C  2.277869823  5.985135279  0.593715826
C  4.431984257  6.069819140  4.458683537
C  4.457636164  5.442456318  1.931751524
H  2.478418937  4.309459376  2.833835245
H  5.732059698  4.432264914  4.739448954
H  3.577945264  4.347581052  0.312950409
H  5.627868814  7.177734396  2.215312312
H  3.473754381  7.093050534  2.837087051
H  2.365233086  7.043711928  0.304098251
H  4.519347520  7.128395790  4.748301112
H  4.632533371  4.394143238  2.218564118

CELL_PARAMETERS (angstrom)
4.308228868  0.169367723  0.000000000
0.724376294  9.618040834  0.000000000
0.000000000  0.000000000  5.052399363

32
pure_bulk_tricycle_ab.xyz
C  1.391729620  0.389191391  0.631328112
C  1.000733314  6.987447110  1.893984336
C  1.231286246  4.122089640  0.631328112
C  1.251528293  3.261678433  1.893984336
C  2.498103591  1.452538668  0.631328112
C -0.074877805  5.895933298  1.893984336
C  0.002509528  5.035504334  0.631328112
C  2.456296749  2.315633015  1.893984336
H  0.405835553  0.889803372  0.631328112
H  1.991997620  6.498792031  1.893984336
H  2.148555660  4.738273041  0.631328112
H  0.321665067  2.661525809  1.893984336
H  3.455766506  0.898446483  0.631328112
H -1.056817085  6.411042488  1.893984336
H -0.863796522  4.351656970  0.631328112
H  3.354857491  2.960754969  1.893984336
C  6.571845558  0.659221779  0.631328112
C  6.181744014  7.257598779  1.893984336
C  6.324242989  4.385592637  0.631328112
C  6.344457326  3.524930042  1.893984336
C  7.648383951  1.749700351  0.631328112
C  5.075931760  6.193480943  1.893984336
C  5.118690522  5.330484557  0.631328112
C  7.572225321  2.610214615  1.893984336
H  5.580498791  1.147677733  0.631328112
H  7.167960893  6.757843805  1.893984336
H  7.253835350  4.986161799  0.631328112
H  5.426966081  2.909224605  1.893984336
H  8.629397222  1.232799188  0.631328112
H  4.117565573  6.746529320  1.893984336
H  4.221080285  4.684114336  0.631328112
H  8.439630645  3.292595467  1.893984336

CELL_PARAMETERS (angstrom)
10.866899534 -1.206231688  0.000000000
-0.470652944  7.454920813  0.000000000
0.000000000  0.000000000  2.525312448

58
defect_G1_4x4x1_chair.xyz
C  0.736457726  1.255110221  7.735497661
C  1.454008823  0.012240059  7.223128880
H  0.776717260  1.240285531  8.843806219
H  1.461130526  0.054540508  6.114810926
C  0.736488133  3.778046644  7.735070688
C  1.443946362  2.516455359  7.242617724
H  0.776871985  3.793024586  8.843374017
H  1.318322923  2.516144619  6.137490277
C  0.722087976  6.295649938  7.650486212
C  1.454042286  5.020720530  7.222373047
H  0.732542761  6.313801559  8.761386659
H  1.461110491  4.978154295  6.114070633
C  0.722054468  8.811753539  7.651086066
C  1.448333380  7.553786598  7.176933828
H  0.732533848  8.793015071  8.761972959
H  1.448161135  7.554007984  6.067376788
C  2.900295446 -0.005749817  7.715451086
C  3.638880788 -1.249184697  7.222571822
H  2.837811994 -0.114455881  8.820588831
H  3.671722082 -1.221591451  6.114250213
C  2.950354067  2.516598270  7.464667355
C  3.653494823  1.298750800  7.492819396
C  2.900359205  5.038836396  7.714807861
C  3.653512917  3.734445771  7.492454388
H  2.837689606  5.147459363  8.819948629
C  2.901081910  7.553604379  7.650464248
C  3.639086271  6.282229263  7.222036294
H  2.879969412  7.553221054  8.761360446
H  3.671992848  6.254755940  6.113731761
C  5.073935331 -1.249139228  7.734818754
C  5.812070299 -2.520518489  7.306738987
H  5.040960243 -1.221723218  8.843120672
H  5.833443199 -2.520503297  6.195829361
C  5.059715125  1.298759374  7.464469100
C  5.812758589 -0.005644334  7.242133736
H  5.875384984 -0.114455464  6.136987153
C  5.059799356  3.734496080  7.464324908
C  5.762904550  2.516620565  7.492447251
C  5.074150273  6.282290510  7.734542653
C  5.813151783  5.038916046  7.242052475
H  5.040887423  6.254618068  8.842833198
H  5.876075198  5.147432088  6.136904162
C  7.264662238 -2.520459577  7.780770463
C  7.991163440 -3.778551853  7.307258364
H  7.264398883 -2.520469102  8.890323523
H  7.980674589 -3.760271986  6.196342280
C  7.258961952  0.012796212  7.734773400
C  7.991035581 -1.262360820  7.307068184
H  7.251550720  0.055274959  8.843079588
H  7.980402249 -1.280980917  6.196152668
C  7.269145486  2.516710312  7.715013602
C  7.976675975  1.255304759  7.222331929
H  7.394304246  2.516378212  8.820192271
H  7.936387106  1.240360110  6.114019099
C  7.259106537  5.021022008  7.735140964
C  7.976773094  3.778175214  7.222787757
H  7.251481867  4.978466637  8.843437335
H  7.936676404  3.793193486  6.114471249

CELL_PARAMETERS (angstrom)
8.724680255 -5.037170382  0.000000000
0.000019458  10.074373300  0.000000000
0.000000000  0.000000000  20.000000000

94
defect_G1_5x5x1_chair.xyz
H  0.012235736  1.464654593  11.388922117
H  1.237288153  0.740601328  8.689914643
H  2.568613840  1.473453497  11.339137389
H  3.770833810  0.777810069  8.621087701
H  5.041933355  1.334699771  11.326610930
H  6.312964329  0.778033682  8.621149299
H  7.515085788  1.473813842  11.339336750
H  8.846421902  0.740504510  8.690118316
H 10.071724605  1.464709492  11.389017124
H 11.348808486  0.727277631  8.717023568
H -1.265126032  3.692020497  11.349048931
H -0.002759387  2.887992238  8.690040166
H  1.298088522  3.674382232  11.339031894
H  2.413089409  2.850961221  8.632832819
H  7.670515714  2.851096925  8.632961244
H  8.785573418  3.674461943  11.339322734
H 10.086256196  2.888117391  8.690141190
H -2.528324438  5.848540677  11.271589513
H -1.265030625  5.045571873  8.612658402
H -0.001884395  5.848625032  11.271448261
H  1.296718202  5.063320666  8.620869143
H  2.414079494  5.885809719  11.326381929
H  7.669310529  5.885772427  11.326591539
H  8.786899229  5.063395767  8.621108255
H -3.768709556  7.996586900  11.271746979
H -2.541782491  7.273182108  8.573486023
H -1.265135581  8.010129145  11.246031467
H  0.011419433  7.273239382  8.573433459
H  1.238390531  7.996771380  11.271543588
H  2.567769936  7.264823452  8.620921161
H  3.771314359  7.958154312  11.339093053
H  5.041866758  7.404052243  8.632772129
H  6.312516732  7.958221740  11.339079473
H  7.516147220  7.264815446  8.621005629
H -5.004953388  10.169341265  11.348882748
H -3.832078524  9.492095596  8.612885601
H -2.505212051  10.184934288  11.271773959
H -1.265150927  9.484262570  8.573529497
H -0.024761122  10.184878080  11.271666847
H  1.302284270  9.492179518  8.612727859
H  2.474547155  10.169317067  11.349036800
H  3.802021396  9.477673096  8.690052322
H  5.042118111  10.176586523  11.388955253
H  6.281622122  9.477651964  8.689877398
C  0.000981307  1.458311668  10.279109577
C  1.257713414  0.731841635  9.800391521
C  2.533835783  1.464764235  10.230498751
C  3.780905355  0.744496030  9.729726079
C  5.041839143  1.455493290  10.221017029
C  6.302834432  0.744565811  9.729773448
C  7.549881958  1.464824841  10.230683204
C  8.826045876  0.731900598  9.800600055
C 10.082806542  1.458387681  10.279208362
C 11.348866605  0.727362325  9.827638146
C -1.265145791  3.649907453  10.239846535
C  0.000135026  2.909965309  9.800513963
C  1.272982068  3.648678474  10.230419902
C  2.518713588  2.911965812  9.738249333
C  3.823470641  3.665336613  9.964523355
C  5.041809755  2.961956340  9.993548579
C  6.260169149  3.665328037  9.964720625
C  7.564969126  2.911994299  9.738412887
C  8.810683481  3.648731722  10.230678703
C 10.083529587  2.910041198  9.800624518
C -2.530568149  5.827342418  10.161075190
C -1.265167980  5.087621416  9.721834374
C  0.000263750  5.827326457  10.160954863
C  1.272719496  5.088786053  9.729494803
C  2.518838171  5.825381840  10.220829376
C  3.823482437  5.072152457  9.993509689
C  5.041819748  5.775548177  9.964553015
C  6.260149418  5.072134960  9.993492750
C  7.564776163  5.825377342  10.220997533
C  8.810921495  5.088823520  9.729727987
C -3.788140492  8.005492398  10.161232542
C -2.531099790  7.279190145  9.683322887
C -1.265118155  8.010099596  10.135327602
C  0.000809411  7.279195651  9.683249116
C  1.257868763  8.005569616  10.161045004
C  2.533666927  7.272873274  9.729554237
C  3.780973412  7.992695802  10.230467092
C  5.041834608  7.282191907  9.738220324
C  6.302731290  7.992682187  10.230438805
C  7.550042901  7.272830148  9.729646902
C -5.041180106  10.190165247  10.239655524
C -3.795962361  9.471235963  9.722080162
C -2.522673584  10.197343753  10.161256792
C -1.265096889  9.471934970  9.683369554
C -0.007489927  10.197376604  10.161142155
C  1.265823966  9.471340748  9.721922279
C  2.510960809  10.190230334  10.239822399
C  3.784350615  9.464365293  9.800539108
C  5.041923718  10.189457371  10.279134804
C  6.299403680  9.464317900  9.800369801

CELL_PARAMETERS (angstrom)
12.613989754  0.000029805  0.000000000
-6.306970142  10.924077318  0.000000000
0.000000000  0.000000000  20.000000000

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defect_G1_6x6x1_chair.xyz
C  0.736692471  1.260939395  7.759672142
C  1.458132407  0.010945832  7.255727816
H  0.752026165  1.231998811  8.869391104
H  1.440117002  0.038014963  6.145992545
C  0.737596248  3.790436285  7.793350643
C  1.464347005  2.532282380  7.317804651
H  0.750211902  3.790402447  8.903336751
H  1.453586822  2.547254539  6.207207901
C  0.736617064  6.319943370  7.759875049
C  1.464289264  5.048678567  7.317894731
H  0.751875119  6.348647181  8.869603049
H  1.453386050  5.033773413  6.207305102
C  0.731874146  8.843706963  7.698122819
C  1.458054562  7.569957299  7.255957078
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H  0.742639194  8.862492068  8.808422092
H  1.439960215  7.542801725  6.146221284
C  0.728713915  11.365298650  7.672637131
C  1.457175386  10.099948887  7.215996266
H  0.732900509  11.365364707  8.783266274
H  1.451090300  10.089150620  6.105864857
C  0.731953188  13.886816302  7.697926572
C  1.457266447  12.630565922  7.215862981
H  0.742777745  13.867966515  8.808224207
H  1.451159828  12.641105174  6.105742811
C  2.923324793  0.006251791  7.696373205
C  3.649151898  -1.253162706  7.222932551
H  2.932289061  -0.007398263  8.807018058
H  3.654478475  -1.243903627  6.112935875
C  2.935361768  2.530046245  7.751634810
C  3.655968643  1.280264117  7.257709105
H  2.966439383  2.523634073  8.860520172
H  3.663039468  1.307799030  6.148758951
C  2.935348606  5.050942528  7.751669239
C  3.647296689  3.790518722  7.259250506
H  2.966517732  5.057165884  8.860546341
H  3.526396562  3.790405790  6.153676918
C  2.923277080  7.574692345  7.696510138
C  3.655947521  6.300759802  7.257830729
H  2.932354613  7.588317845  8.807148772
H  3.662919727  6.273151218  6.148904907
C  2.917187681  10.101722466  7.672792229
C  3.649049121  8.834122082  7.223060334
H  2.915106623  10.105474002  8.783425044
H  3.654311419  8.824980611  6.113059889
C  2.917277950  12.628820130  7.672658476
C  3.648753413  11.365233044  7.215976141
H  2.915129780  12.625280256  8.783291165
H  3.661043659  11.365181650  6.105850050
C  5.102732684  -1.251995703  7.696373939
C  5.839366641  -2.518566698  7.255750778
H  5.086408527  -1.251036084  8.807011173
H  5.871772407  -2.520724277  6.146018955
C  5.104507759  1.267719363  7.747003918
C  5.839682463  0.019518507  7.257739645
H  5.045818373  1.166043528  8.853002511
H  5.860066812  0.039294329  6.148785943
C  5.154057088  3.790595592  7.486556688
C  5.857594539  2.572097141  7.516010725
C  5.104490410  6.313410407  7.747123335
C  5.857596316  5.009058971  7.516214361
H  5.045626894  6.415219612  8.853077743
C  5.102683119  8.832994689  7.696433360
C  5.839665210  7.561531369  7.257731103
H  5.086374258  8.832041849  8.807072943
H  5.859922375  7.541572728  6.148795077
C  5.099359983  11.365292136  7.698039959
C  5.839338217  10.099541541  7.255818397
H  5.077697337  11.365430696  8.808336116
H  5.871741798  10.101609835  6.146079202
C  7.282640910  -2.518325622  7.759622287
C  8.022869101  -3.784307040  7.318584379
H  7.250004942  -2.519469749  8.869336360
H  8.045487305  -3.784368321  6.208291390
C  7.282339171  0.020337855  7.751650648
C  8.019795419  -1.252479264  7.317728321
H  7.261394044  0.044093170  8.860552560
H  8.038051702  -1.254319068  6.207141708
C  7.264614739  2.572043669  7.486656667
C  8.017944078  1.267122857  7.259211415
H  8.078363677  1.162320248  6.153595552
C  7.264576375  5.009122014  7.486471755
C  7.968073561  3.790601311  7.516030912
C  7.282373223  7.560718102  7.751492174
C  8.018018045  6.313955725  7.259078787
H  7.261275310  7.536897897  8.860364882
H  8.078550551  6.418663355  6.153496056
C  7.282626410  10.099330673  7.759678551
C  8.019797722  8.833534964  7.317712734
H  7.250063312  10.100456745  8.869402195
H  8.038164286  8.835466570  6.207120715
C  9.473153262  -3.784292223  7.801974157
C 10.204913823  -5.047759380  7.345218662
H  9.460334481  -3.784278752  8.912093645
H 10.207312662  -5.043726546  6.234614892
C  9.472814917  -1.252759803  7.793161504
C 10.204955162  -2.520878830  7.345178680
H  9.466456311  -1.241910694  8.903133430
H 10.207332942  -2.524932007  6.234579400
C  9.465490327  1.280750839  7.751641425
C 10.199078530  0.005712869  7.317738704
H  9.455432995  1.310778373  8.860541652
H 10.191516532  -0.011071526  6.207157128
C  9.474217873  3.790509132  7.747055585
C 10.187548346  2.529710213  7.257757419
H  9.591647265  3.790414945  8.853065522
H 10.160143148  2.521933482  6.148815200
C  9.465549131  6.300232244  7.751550002
C 10.187610025  5.051244758  7.257725183
H  9.455390706  6.270082918  8.860435798
H 10.160210172  5.058976124  6.148781086
C  9.472790957  8.833753676  7.793223223
C 10.199093570  7.575288448  7.317707078
H  9.466505297  8.822808857  8.903211843
H 10.191541934  7.592160040  6.207112665
C 11.664967247  -5.049839964  7.802014833
C 12.390159866  -6.305786228  7.318590406
H 11.671374995  -5.060986852  8.912131470
H 12.378935641  -6.286126206  6.208293984
C 11.664969610  -2.518956438  7.802067367
C 12.393291617  -3.784393526  7.345299050
H 11.671200502  -2.507902541  8.912187700
H 12.388722247  -3.784302110  6.234689659
C 11.663869465  0.011136658  7.759673238
C 12.390125303  -1.262967440  7.318708574
H 11.681081138  0.038856458  8.869380079
H 12.378867669  -1.282602930  6.208406414
C 11.657188339  2.532185611  7.696364769
C 12.385720611  1.260910109  7.255778343
H 11.664563787  2.546818427  8.806999010
H 12.371386671  1.231713922  6.146042598
C 11.657226076  5.048748836  7.696356644
C 12.384975263  3.790467411  7.222903091
H 11.664596283  5.034128079  8.806997331
H 12.374302195  3.790406899  6.112908920
C 11.663913966  7.569762288  7.759602592
C 12.385747718  6.319977694  7.255702490
H 11.681184130  7.542037174  8.869318454
H 12.371313612  6.349104138  6.145973717

CELL_PARAMETERS (angstrom)
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0.000005441  15.149605620  0.000000000
0.000000000  0.000000000  20.000000000

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defect_G1_7x7x1_chair.xyz
C  0.004567327  1.456780314  10.194794007
C  1.259302284  0.731570427  9.707087532
C  2.525150321  1.459276535  10.163008954
C  3.789787135  0.731399367  9.703857728
C  5.045571105  1.457286106  10.187499984
C  6.318642364  0.730135257  9.747329262
C  7.570306399  1.454005040  10.245294043
C  8.843830478  0.726513824  9.807230391
C 10.098652897  1.452846288  10.292471938
C 11.364438799  0.724158272  9.838183381
C 12.629004836  1.452506726  10.296642538
C 13.884893049  0.726683802  9.813223544
C 15.157971220  1.453265928  10.254547089
C 16.409676286  0.730538333  9.754858151
C -1.254399588  3.644643195  10.256826748
C -0.004427936  2.923009729  9.752771891
C  1.267185165  3.651105415  10.192557421
C  2.524317588  2.923850266  9.714861512
C  3.783399108  3.651287800  10.186658934
C  5.053569405  2.922892200  9.743095063
C  6.304381008  3.645095650  10.244071564
C  7.578014211  2.919100067  9.801410434
C  8.833707134  3.644038966  10.286125057
C 10.102540289  2.914586541  9.838732937
C 11.363637246  3.643896520  10.305145840
C 12.626688940  2.914646395  9.844250682
C 13.894167825  3.643749201  10.296548379
C 15.150749100  2.919045933  9.813273355
C -2.518631459  5.835286817  10.289196919
C -1.259177534  5.109540251  9.815680866
C  0.015333270  5.842529317  10.252212084
C  1.263954218  5.121338794  9.756191792
C  2.525470565  5.833773516  10.244351542
C  3.784762999  5.121441710  9.749886908
C  5.035064401  5.842630942  10.241467433
C  6.308904198  5.109916587  9.802752084
C  7.568225453  5.835135970  10.276552932
C  8.836317235  5.103142572  9.827360216
C 10.098608383  5.834677186  10.286746653
C 11.364702306  5.100739633  9.838905406
C 12.628784252  5.834823668  10.292684886
C 13.892722743  5.103081333  9.838201202
C -3.783970212  8.024984417  10.254554047
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H  8.758442829  21.884866905  16.931804470
H  9.087884950  20.112215967  15.682655121
H  7.426417281  17.889619342  16.906424902
H 10.687124487  16.330346238  15.692883167
H  5.734218587  21.479748023  16.915528048
H  6.107813377  19.444118084  15.673310795
H 10.442353719  18.358058767  16.995936181
H  7.536073023  16.246251321  18.124316389
H  8.751138344  21.891532903  19.427816065
H  9.075436796  20.090617915  18.191525733
H  7.384622620  17.892022377  19.420374599
H 10.585840367  16.241259016  18.196556734
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