Nonlinear transport through ultra-narrow zigzag graphene nanoribbons: non-equilibrium charge and bond currents

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Abstract
The electronic nonlinear transport through ultra-narrow graphene nanoribbons (sub-10 nm) was studied. A stable region of negative differential resistance (NDR) appears in the $I$–$V$ characteristic curve of odd zigzag graphene nanoribbons (ZGNRs) at both positive and negative polarity. This NDR originates from a transport gap induced by a selection rule that blocks the electron transition between disconnected energy bands of ZGNR. Based on this transition rule, the on/off ratio of the current increases exponentially with ribbon length up to $10^5$. In addition, charging effects and the spatial distribution of bond currents were studied by using the non-equilibrium Green’s function formalism in the presence of electron–electron interaction at a mean-field level. We also performed an ab initio density functional theory calculation of the transmission through a passivated graphene nanoribbon to demonstrate the robustness of the transport gap against hydrogen termination of the zigzag edges.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction
Graphene is a two-dimensional (2D) carbon that has been explored recently [1]. Experiments on graphene-based devices [2] have shown the possibility of controlling their electrical properties by using the edge structure and the application of an external gate voltage. Nowadays, by using a chemical method [3], it is possible to fabricate field effect transistor graphene nanoribbons (GNRs) with ultra-narrow widths and smooth edges, which are possibly well-defined zigzag or armchair edge structures. A useful transport gap is opened in sub-10 nm GNRs at room temperature, which results in a high on/off current switching up to $10^6$. The origin of the transport gap can be understood by using two factors: the suppression of transport due to edge disorder leading to Anderson localization, and confinement along the transverse direction [4, 5]. In addition to these factors, in ultra-narrow zigzag graphene nanoribbons (ZGNR), the flow of current is also blocked by symmetric selection rules [6–12].

Negative differential resistance (NDR) [13] in nanoelectronic devices has also been observed in metallic nanotube junctions [14] and, in the case of potential barriers, in 2D graphene sheets [15].

In this paper, to shed light on the experimental work of [3], we study nonlinear transport in odd ZGNRs by using the non-equilibrium Green’s function (NEGF) formalism. It is shown that a stable NDR against electrostatic interaction up to $10^5$ appears in ultra-narrow ZGNRs around $\pm t$ at both positive and negative polarity, where $t$ is the hopping integral between carbon atoms. The on/off ratio of this NDR increases exponentially with ribbon length. The NDR phenomenon occurs in the far-from-equilibrium regime.

Although parity is not conserved in odd ZGNRs, current reduction is induced by another selection rule in which transition between disconnecting band groups is forbidden (Cresti et al [6]). The edges of graphene ribbons can also simply absorb some chemical compounds [16]. It is
demonstrated that this NDR is not very sensitive to the asymmetry of the ribbons, whereas a transport gap in even ZGNRs that is based on the reflection symmetry is completely destroyed due to edge disorder. The above-mentioned selection rule is valid for both even and odd ZGNRs, whereas parity selective tunneling just belongs to even ZGNRs. This transport gap is robust against hydrogen termination. In addition to the model calculation, using the TranSIESTA code [25], we performed an ab initio density functional theory (DFT) calculation of the transmission through a GNR with hydrogen termination of zigzag edges. The results of first-principle calculation confirms that the transport gap originates from the transition rule between disconnected bands.

This NDR is stable against the presence of electron–electron (e–e) interaction at a mean-field approximation. It is concluded from self-consistent charge and potential profiles that the external potential is screened by charge redistribution around the contact junctions so the potential profile deep inside the ribbon remains flat. Furthermore, the e–e interaction increases the on/off ratio of the current. Moreover, at low and high applied biases, we study the spatial profile of local currents in the presence of e–e interaction, which contrasts with the non-equilibrium charge profile.

This paper is organized as follows. We explain the Hamiltonian and present a short review of the NEGF formalism in section 2. In section 3, we present our results concerning NDR in the I–V curve and charging effects in high applied bias and spatial bond currents. We then present the results of an ab initio calculation using the TranSIESTA code. Finally, we present the conclusions.

2. Formalism

The single-electron Hamiltonian of the molecule is defined as

\[
H[n] = \sum_{i=1}^{2N \times M} \left[ \varepsilon_i + u^{\text{ext}}_i + \sum_{j=1}^{2N \times M} V_{ij} \delta n_i \right] c_i^{\dagger} c_i + \sum_{\langle ij \rangle} I(c_i^{\dagger} c_j + c_i c_j^{\dagger}),
\]

where \( c_i^{\dagger} \) and \( c_i \) are the electron creation and annihilation operators, respectively. \( 2N \times M \) and \( t \) are the number of atomic sites and the hopping energy between nearest-neighbor atoms. One \( \pi \) orbital is considered per site for graphene as a planar 2D system. Without loss of generality, we set onsite energies \( \varepsilon_i \) of all sites to be equal to zero. All energies and voltages are in units of \( t = 2.7 \text{ eV} \). The Fermi energy of an undoped graphene nanoribbon is at half-filling \( E_F = 0 \) due to perfect electron–hole symmetry. By applying a source–drain bias, the site energies are shifted by a linear potential distribution along the molecule \( u^{\text{ext}}_i \) which is the solution of the Laplace equation. The applied bias \( V \) is divided symmetrically on the left and right electrodes as \(-V/2 \) and \( V/2 \), respectively. \( V_{ij} \) is the electrostatic Green’s function and \( \delta n_i = n_i - n^{0}_i \) is the change in the self-consistent charge \( n_i \) from its value in zero source–drain voltage, \( n^{0}_i \). This third term is the direct Coulomb interaction created by the source–drain bias-induced charges. It includes the Hartree term that is the solution of the Poisson equation and is located on the diagonal terms of the Hamiltonian. To calculate the electrostatic Green’s function, we have used the method explained in [17] and its appendix (see also the references in [17]).

To make this section self-containing, we present a very brief review of the NEGF formalism. Charge density in the non-equilibrium situation is calculated by using \([-i G^{-1}] \) as the occupation number in the presence of two electrodes with an applied source–drain bias [18]:

\[
n_i = -\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Im}(G^{a}_{E}(E))_{ii} dE + n^{\text{non-eq}}_i,
\]

(2)

where the non-equilibrium part of charge can be calculated by using the following integral:

\[
n^{\text{non-eq}}_i = \frac{1}{2\pi} \int_{E_F^{L} - (V/2)}^{E_F^{R} + (V/2)} [-i G^{a}_{E}(E)]_{ii} dE,
\]

(3)

where within a one-particle theory,

\[
-i G^{c} = G^{-1}(\Gamma^{a}_{L} f_{L} + \Gamma^{a}_{R} f_{R}) G^{a}.
\]

(4)

Here \( f_{L/R} \) is the Fermi–Dirac distribution function of electrodes and \( G^{c/a} \) is the retarded/advanced Green’s function defined as

\[
G^{c/a}_{\eta} = [(E \pm \eta) I - H[n] - \Sigma^{r/a}_{L} - \Sigma^{f/a}_{R}]^{-1}
\]

(5)

and \( \Gamma \) is the escape rate of electrons to the electrodes, which is related to the self-energies as \( \Gamma_{\eta} = i[\Sigma^{c}_{\eta} - \Sigma^{a}_{\eta}] \), with \( p = L/R \) (see chapter 2 and references [20]). Here \( \eta \to 0^{\pm} \). Solving equations (2) and (5) self-consistently results in a self-consistent charge and Green’s functions. Finally, the current passing through the molecule is calculated by the Landauer formula for zero temperature [19], which is valid for coherent transport:

\[
I(V) = \frac{2e}{h} \int_{E_F - V/2}^{E_F + V/2} dE T(E, V),
\]

(6)

where \( T(E, V) \) is the bias-dependent transmission coefficient:

\[
T = \text{Tr}[G^{c} \Gamma^{a}_{L} G^{a} \Gamma^{c}_{L}].
\]

(7)
Figure 2. The current–voltage characteristic curve of an odd ZGNR with \( N = 5 \) (zigzag chains). \( I–V \) curves are presented for two ribbon lengths: \( M = 5 \) and 10. For the case of \((M, N) = (5, 5)\) and for comparison purposes the \( I–V \) curve is also plotted in the presence of e–e interaction \((U)\) and the asymmetric factor \((\epsilon_w)\).

Figure 1 shows a ZGNR with an odd number of zigzag chains in width \((N)\). The central interacting region and the left and right electrodes are the three regions of the ribbon. Odd ZGNRs have a bisection plane whose intersection with the ribbon has been shown as the x-axis in figure 1. Although this plane bisects the ribbon, it is not a reflection plane. If the upper half of the ribbon is displaced by \(a/2\) with respect to the lower one, mirror symmetry is achieved against the \(x\)-axis. \( a \) is the bond length of \(C–C\). In other words, the part of the wave function that is a functional of the \(y\) variable is an eigenvector of the parity operator \([21]\).

3. Results

The current–voltage characteristic curve of an odd ZGNR with five zigzag chains \((N = 5)\) is shown in figure 2. Below the external bias \(1.2t\), the current increases linearly with the applied bias as in an ohm device. After a threshold voltage \((1.2t)\), NDR occurs at both positive and negative polarity.

The origin of the NDR seen in odd ZGNRs is interpreted by analyzing their energy spectrum and the transmission curve. Figure 3 shows the energy spectrum \(E(n, k_x)\) and the transmission through a 5-ZGNR at \(V = 1.4t\). Note that \(n\) is the number of bands from the bottom \((n = 1)\) to the top of the band structure \((n = 2N)\) and \(k_x\) is the longitudinal momentum.

In odd ZGNRs, parity has a non-commutative relation with the Hamiltonian. Therefore, parity has no conservation, and consequently transmission is not blocked by the parity selection rule, while parity conservation in even zigzag nanoribbons opens a transmission gap around the Fermi level \([12]\). In the range \(BC\) of figure 3, there exists one conducting channel that results in unity transmission around the Fermi level. In this range, electrons that occupy \(-k\) states of the lower band of the central band group (the dashed blue bands) belonging to the right electrode are injected into the unoccupied \(-k\) states of the upper band of the central group belonging to the left electrode. So at low biases, the current increases linearly with the bias. This single-channel transport around the Fermi level remains unchanged even for high voltages. However, for voltages greater than the NDR threshold voltage \((V > V_T)\), the blocked regions marked by the ranges \(AB\) and \(CD\) come into the current integration window. The current integration window, based on equation (6) and \(E_T = 0\), is proportional to \(V_{SD}\) and is shown by the bold hollow arrows in figure 3. Therefore, when the source–drain applied bias increases, the current begins to decrease.

Blocked regions \((AB\) and \(CD\)) arise from a selection rule that increases backscattering in the lengthy ribbons. According to this rule, electron transition between those bands that are disconnected from the viewpoint of longitudinal momentum decreases exponentially with length. The topology of zigzag graphene ribbons divides the band structure into three different groups \([6]\). The three groups, called the upper \((n = 1, 2, 3, 4)\), central \((n = 5, 6)\) and lower \((n = 7, 8, 9, 10)\) groups, are classified based on the bands that are connected in terms of \(k_x\). The variation in the momentum of electrons passing through the system strongly depends on the smoothness or sharpness of the potential. The transition probability of electrons with the \(k\) state injected by the right electrode into the \(q\) state as an empty state in the left electrode is proportional to the Fourier transform of the longitudinal voltage \([6]\) as \(\langle \psi(k) | V | \psi(q) \rangle \propto \tilde{V}(k - q)\). So a smooth variation in potential in the longer ribbons results in a small variation in the momentum of electrons. Consequently, a smooth potential in the longitudinal direction can just scatter electrons into those states belonging to the energy bands that are connected from the viewpoint of momentum \([6, 12]\).

The bias dependence of transmission leads us to plot a contour of the transmission in the plane of energy and applied bias as shown in figure 4. In this figure, the solid lines show the current integration window. Moreover, the dashed lines clarify the regions \(AB\) and \(CD\) corresponding to the transport gaps shown in figure 3. The intersection of these blocked regions and also the current integration window would be around \(1.2t\), which is the threshold voltage \(V_T\) for the current reduction.

Band structure analysis demonstrates that the threshold voltage is equal to the half-width of the central bands at \(k_x = 0\) as \(V_T \geq \delta = \{E(N + 1, k_x = 0) - E(N, k_x = 0)\}/2\). As shown in figure 3, \(\Delta\) is the energy separation of the upper bands from the central bands at the Dirac points. There is a log-normal behavior of \(\delta\) versus the number of zigzag chains \((N)\) such that as \(N \to \infty\), the NDR threshold voltage asymptotically approaches the value of \(0.9738 \pm 0.0002t\). So the NDR threshold voltage slightly decreases with the ribbon width.

Analysis of the transport gaps appearing in the band structure shows that they are equal to \(\Delta - \delta + V_{SD}\), where \(\Delta \propto N^{-1}\). Since \(\delta\) approaches a constant value as \(N \to \infty\), at a given voltage, the transport gap disappears for \(N > 30\), which is nearly equivalent to 10 nm.

Another factor that enhances the performance of this electronic switch is ribbon length. Figure 2 shows the increase of the on/off ratio as a function of ribbon length. Moreover, the NDR region \((V_{off} - V_{on})\) occurs in a more extended range of the \(I–V\) curve. The exponential decay of transmission with length in the gap regions develops the quality of switching. It
Figure 3. Energy spectrum of the left and right electrodes and the transmission through a ZGNR with \((M, N) = (10, 5)\) at voltage \(V_{SD} = 1.4t > V_T\). The band structure is divided into three groups: the upper, central and lower band groups. These groups are classified based on the bands that are connected in terms of \(k_x\). The bold hollow arrows show the current integration window that, based on equation (6), is proportional to \(V_{SD}\). The Fermi level is set to be \(E_f = 0\). The half-width of the central bands at \(k_x = 0\) is called \(\delta\), which is equal to the threshold NDR voltage. \(\Delta\) is the energy separation of the upper bands from the central bands at the Dirac points. The transport gaps \(\Delta_{\delta}A\) and \(\Delta_{\delta}D\) are equal to \(\Delta - \delta + V_{SD}\).

Figure 4. Contour plot of transmission versus energy and applied bias for a GNR with five zigzag chains in width and 10 unit cells in length. Dark solid lines show the current integration window and white dashed lines show the forbidden region for electron transition from the band groups of the upper or lower bands to the bands of the central group.

is shown in figure 5 that \(I_{on}/I_{off}\) increases exponentially with ribbon length.

Another parameter that affects the \(I-V\) curve is e–e interaction. In this case, interaction intensifies the NDR effects such that the off-current decreases as compared with the non-interacting system and also the NDR region becomes more extended.

Figure 5. The exponential increase of the on/off current ratio as a function of ribbon length \((M)\).

If one of the ribbon edges is doped by a small impurity such as \(\epsilon_\alpha = 0.1t\), because of a band gap that is induced by the edge impurity at the band center, the current at low biases decreases. Figure 2 shows that even in the presence of edge impurity, still the region containing NDR exists. However, asymmetry decreases the on/off ratio of the current. Furthermore, an asymmetric ZGNR behaves as a semiconductor, while symmetric ZGNRs behave as ohmic devices [23]. The effect of asymmetry on NDR competes with the ribbon length. Since asymmetry cannot be ignored
in experiments, longer ribbons are in favor of keeping NDR in the $I-V$ curve.

On the other hand, in addition to edge impurity, this asymmetry can be assigned to the sublattice symmetry breaking induced by spontaneous ferromagnetic spin ordering of the electrons localized at the zigzag edges [22]. In fact, the border atoms at the two opposite zigzag edges belong to different sublattices. So spin orientation along the edges induces different magnetic potentials at the edges. As a result, a small band gap is opened around the Fermi level that, depending on the ribbon width, is about 0.15 eV. The asymmetry we have considered is about 0.3 eV, which is stronger than the gap opened by spin polarization of the edges. We can conclude that spin polarization along the zigzag edges cannot affect the emergence of this NDR phenomenon [23].

3.1. Charging effects

To understand why details of the electrostatic potential do not affect the emergence of NDR, we compare transmission in the presence and absence of e–e interaction. Figure 6 compares the transmission curve for the voltage of 1.2$t$ at the NDR threshold $V_T$ and that for a larger value such as 1.5$t$.

It is clear that for voltages lower than the NDR threshold, transmission in the conducting region $BC$ is robust against e–e interaction. However, for voltages $V > V_T$, transmission in the conducting region $BC$ decreases with e–e interaction. This is the reason for the decrease of off-current in the presence of e–e interaction. Furthermore, the transmission curve in the blocked regions $CD$ and $AB$ exhibits a small enhancement with e–e interaction for the entire range of voltages.

To elucidate the physics behind the robustness of the NDR phenomenon against e–e interaction, we investigate the self-consistent potential profiles shown in figures 7(a) and (b). In fact, the external potential is well screened by charge redistribution so that the potential mostly drops at the contact junctions. This fact is represented in figure 7. So, the electrostatic potential of atoms located far away from contact junctions (deep inside the ribbon) remains nearly flat. In more detail, the depletion in charge close to the source electrode reduces the source potential as $U \delta n$. Therefore, source the potential cannot penetrate the central part of the system. On the opposite side of the system, charge is accumulated close to the drain electrode such that the decreasing of the potential is weakened.

It is useful to investigate the bias dependence of the total transferred charge from/into the system. Figure 7(c) shows that the transferred charge, in comparison to its neutrality point value ($n_0$ with zero source–drain applied bias), decreases for voltages higher than the NDR threshold, whereas it remains unchanged for voltages $V < V_T$. In other words, for $V < V_T$, the in-flowing and out-flowing charges balance each other, while for $V > V_T$, the system becomes devoid of charge. It can be seen that the threshold voltage for the depletion of charge is correlated with the NDR threshold voltage. This behavior is very similar to what is seen in graphene nanojunctions [17]. As a consequence, at high voltages, due to the accumulation of charge close to the drain electrode, the external potential is always screened in the middle of the graphene strip. The screening effect induces a sharp variation in electrostatic potential at the contacts, which enhances the transition probability between disconnected band groups. Therefore, transmission in the blocked regions ($CD$ and $AB$) increases in comparison to the non-interacting system. However, blocked regions have no contribution in the current calculation.

3.2. Spatial distribution of bond currents

Charge conservation based on the continuity equation yields non-equilibrium bond charge current [24] for a non-interacting tight-binding Hamiltonian:

$$ J_{ij} = \frac{2e}{h} \int_{E_{i}-(V/2)}^{E_{i}+(V/2)} [G_{ij}^{-}(E) - G_{ji}^{-}(E)] \, dE, $$

where sites $i$ and $j$ are nearest-neighbor atoms whose hopping integral is non-zero. Now, the charge continuity equation is derived by using the Heisenberg equation:

$$ e \frac{d}{dt} n_{i}^{\text{non-equil}} + \sum_{j} [J_{ij} - J_{ji}] = 0, $$

where $j$ is the nearest-neighbor atomic site around the $i$th atomic site. It can be simply proved that the integrands in equations (3) and (8) are real. In fact, the transpose of the matrix $-iG^{\pi}$ in equation (4) is equal to its conjugate. So, diagonal terms of $-iG_{ij}^{\pi}$ and also the terms of $G_{ij}^{\pi} - G_{ji}^{\pi}$ are real.

The bond charge current formulated in equation (8) has been derived for the non-interacting tight-binding Hamiltonian. However, by using the Heisenberg equation, it can be simply proved that this formula is still applicable for the Hamiltonian described in equation (1) in which a Hartree interaction appears on diagonal elements of the Hamiltonian. On the other hand, charging effects originating from electrostatic interaction (Hartree term) adjust local currents by means of a lower Green’s function. Figure 8 (top) shows the spatial profile of the local current at each site. In the center of the ribbon, the magnitude of local current densities is larger than that in the zigzag edges of the ribbon.
Figure 7. (a) Self-consistent charge profile at 1.5t. The charge compared with its neutrality point $n_0$ when there is no applied bias. The transferred charge is equal to $n - n_0$. The electrostatic potential profile is calculated according to this transferred charge. (b) Averaged electrostatic potential variation on the unit cell as a function of the ribbon axis. (c) Total transferred charge from/into the ribbon as a function of source–drain voltage.

This feature is valid for both ranges of low and high voltages not more than 1.5t. The reason can be seen by looking at single-channel transport through a ZGNR even for high voltages [24]. One-channel transport is an indirect result of the transition rule in which transition between disconnected bands is forbidden. For voltages higher than 1.5t, the alignment of local currents along the ribbon axis is gradually disturbed.

In contrast to the local current distribution, as shown in figure 8 (bottom), non-equilibrium charge reaches its maximum at the ribbon’s edges. This result is compatible with the continuity equation (9) so that atomic sites with larger local current correspond to smaller non-equilibrium charge. On the other hand, non-equilibrium charge increases for atomic sites with higher onsite energy due to applied bias (close to the source electrode), while its value tends to zero for sites close to the drain electrode.

3.3. Comparison of odd and even ZGNRs

There are some interesting differences between the results arising from odd ZGNRs and those belonging to even ZGNRs [12], which is a kind of odd–even effect. Here, NDR appears at voltages higher than 1t, whereas in an even ZGNR, NDR occurs at voltages lower than 1t. The on/off ratio of the current in gated even ZGNRs increases as a power law with the ribbon length, whereas here, the on/off ratio increases exponentially. The screening of the external bias by electrons of a system of even ZGNRs is therefore stronger than screening effects in odd ZGNRs. As a consequence, in even ZGNRs the effect of electrostatic interaction on the increase in on/off ratio is much stronger than that in odd ZGNRs. Furthermore, transferred charge from/into the central portion of the GNR depends on odd or even zigzag chains in width.

4. Hydrogen-terminated nanoribbon

To show how passivation of zigzag edges of a GNR affects transport properties, we compare the results of the presented model with the transport properties calculated using the TranSIESTA code [25]. This code is based on the DFT approach. We have used the following options to calculate the SIESTA code: the generalized gradient approximation with the Perdew–Burke–Ernzerhof exchange-correlation functional [26], double-ζ plus polarization orbital bases for all atoms, and the Troullier–Martins norm-conserving pseudopotentials to represent the cores, 200 Ry real space mesh cut-off for charge density and a supercell within 20 Å of vacuum between the periodic GNRs.

Figure 9 (top) shows a schematic view of an odd ZGNR that is saturated by hydrogen atoms. Transmission around the Fermi energy is represented in figure 9 (bottom). The energy scale is shifted so that the Fermi energy of the system, if there is no bias voltage, is zero ($E_F = 0$). When there is a finite bias, the Fermi energy of the left electrode is placed at $V/2$ and that of the right electrode at $-V/2$. The occupation number on atoms in the central part of the system is determined by $\langle -iG^< \rangle_l$.

As is clear from figure 9 (bottom), there exists one transmitting channel for each spin around the Fermi energy level. This result is in complete agreement with the band structure analysis shown in section 3. There exists only one
transmitting channel in the region $BC$ presented in figures 3 and 4. The transport gap in figure 9 (bottom) begins to open at a voltage of about $1.2 \, \text{eV} \simeq 0.5t$ and for an energy of about $2.7 \, \text{eV} \simeq t$. These points correspond to the points marked by the cross sign in figure 4 in which the transport gap begins to open as the applied bias increases. As a result, we demonstrate that the transport gap that is responsible for the emergence of the NDR phenomenon could also open in GNRs with passivated zigzag edges.

5. Conclusion

In conclusion, based on a model calculation of the NEGF formalism, we found that there exists a region of NDR in the $I-V$ curve of ultra-narrow (lower than 10 nm) ZGNRs with an odd number of zigzag chains in width. This NDR is induced by a transport gap that originates from electron transition between disconnected bands of energy from the viewpoint of longitudinal momentum. The on/off ratio of the current exponentially increases up to $10^5$ as a function of ribbon length, which suggests the possibility of manipulation of odd ZGNRs as a high-quality switch in nanoelectronics based on GNRs. In addition, $e-e$ interaction enhances the on/off ratio of the current that originates from a flat electrostatic potential deep inside the ribbon due to the screening of the external bias by electrons close to the junctions. By using the continuity equation, the spatial profile of local currents is calculated in the presence of Hartree electron interactions. In both high and low biases, the local current reaches its maximum values in the center of the ribbon, while in contrast to the local current profile, non-equilibrium charge has its maximum values at the edges of the ribbon. Furthermore, this NDR is not very sensitive to the edge asymmetry. So the emergence of this NDR is robust against spin orientation along the edges.

By using $ab$ initio DFT, we also show that the transport gap that is responsible for the emergence of NDR exists in GNRs passivated by hydrogen atoms.

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