Growth Mechanism of SiC Chemical Vapor Deposition: Adsorption and Surface Reactions of Active Si Species

Pitsiri Sukkaew, Emil Kalered, Erik Janzén, Olle Kordina, Örjan Danielsson and Lars Ojamäe

The self-archived postprint version of this journal article is available at Linköping University Institutional Repository (DiVA):
http://urn.kb.se/resolve?urn=urn:nbn:se:liu:diva-144885

N.B.: When citing this work, cite the original publication.

Original publication available at:
https://doi.org/10.1021/acs.jpcc.7b10751

Copyright: American Chemical Society
http://pubs.acs.org/
Growth Mechanism of SiC CVD – Adsorption and Surface Reactions of Active Si Species

Pitsiri Sukkaew*, Emil Kalered, Erik Janzén, Olof Kordina, Örjan Danielsson and Lars Ojamäe*.

Department of Physics, Chemistry and Biology, Linköping University, SE–581 83 Linköping, Sweden.

ABSTRACT

Silicon carbide is a wide bandgap semiconductor ideally suitable for high temperature and high power applications. An active SiC layer is usually fabricated using halide-assisted chemical vapor deposition (CVD). In this work, we use quantum chemical density functional theory (B3LYP and M06-2X) and transition state theory to study adsorptions of active Si species in the CVD process on both the Si face and the C face of 4H-SiC. We show that adsorptions of SiCl, SiCl₂, SiHCl, SiH and SiH₂ on the Si face likely occurs on a methylene site, CH₂(ads), but the processes are thermodynamically less favorable than their reverse or desorptions. Nevertheless, the adsorbed products become stabilized with help of subsequent surface reactions to form a larger cluster. These cluster formation reactions happen with rates that are fast enough to compete with the desorption processes. On the C face, the adsorptions likely occur on a surface site terminated by a dangling bond, *(ads), and produce the products which are thermodynamically stable. Lastly, we
present the Gibbs free energies of adsorptions of Si atoms, SiX, SiX₂, SiHX, for X being F and Br. Adsorptions of Si atoms are shown to be the most thermodynamically favorable among all the species in the study. Among the halide-containing species, the Gibbs free energies (Δ\textsubscript{R}G\textsuperscript{o}) from smallest to largest are observed in the adsorptions of SiX, SiHX and SiX₂, for X being the halides. The results in this study suggest that the major Si contributors in SiC-CVD process are Si atoms, SiX (for X being the halide) and SiH.

**Introduction**

Silicon carbide (SiC) is a wide bandgap semiconductor ideally suitable for high-voltage, power devices \(^1\textsuperscript{-3}\) and sensors\(^4,5\). Among SiC numerous polytypes, the 4H polytype is a common choice for electronic applications \(^6\) thanks to its superior characteristics of high breakdown electric field and high mobility \(^1\). An active layer of 4H-SiC is usually fabricated using chemical vapor deposition (CVD). The process is performed at temperatures ~1500-1600 °C and pressures ~50-300 mbar, typically using a mixture of silane (SiH\(_4\)) and light hydrocarbons diluted in the flow of hydrogen. Addition of halides, especially chlorine, is often used to suppress the formation of silicon clusters in the gas phase so that the growth rate can be increased by increasing the precursor concentration \(^7,8\). It has been shown recently that Br chemistry worked similarly well in terms of material qualities and growth rates \(^8\). In addition, F-chemistry was also reported to produce high quality SiC homoepitaxial layer \(^9\).

CVD processes involve chemical reactions in the gas phase and on the surface. During the process, active species are produced from pyrolysis before transported to the surface and become incorporated into the growing layer. For the F-, Cl- and Br-assisted SiC-CVD conditions, it was shown using thermodynamic equilibrium calculations \(^8,10\) that the Si species with the highest gas
phase concentrations are SiX, SiX₂, SiHX (for X referring to F, Cl and Br) as well as Si₂C and Si atoms. This suggests that these species might act as the Si growth contributors.

Surface reactions of SiH₂, SiCl₂ and SiBr₂ were recently reported⁸,¹¹ on the C-face of 4H-SiC. It was shown that SiCl₂ and SiBr₂ behave similarly for the reactions considered⁸. This suggests that similar reactivity may be expected among different halides. In our recent study, we compare SiF, SiHF and SiF₂ adsorptions on the Si-face of 4H-SiC and found that SiF was the most active species in the set, while SiF₂ was the least active species¹⁰. These studies¹⁰,¹¹ also showed that at the CVD process temperature, most adsorptions occurred with relatively large, positive Gibbs free energies (ΔR G°). This means that adsorption is less favorable than its reverse.

In our previous work¹², we presented growth mechanisms of 4H-SiC with the focus on active C-species adsorptions and their subsequent surface reactions on the Si-face of 4H-SiC. We showed that hydrocarbon adsorptions occurred with much slower rates than desorptions, but with help of subsequent reactions, the process proceeded forward and produced stable final products. In this work, we continue with adsorptions of active Si-species and their subsequent reactions on both the Si face and the C face. We consider the following Si-species: SiH, SiH₂, SiCl, SiHCl, and SiCl₂. The adsorption sites on the Si face are CH₃(ads), CH₂(ads) and C₂H₄(ads), as shown in Fig. 1a-c. We have shown in our previous work¹² that these three surface sites can be produced from adsorptions (and subsequent reactions) of gaseous CH₃, C₂H₂ and C₂H₄ respectively. On the C face, we consider two adsorption sites: H(ads) and *(ads), referring respectively to a surface site (C site) terminated by a hydrogen atom and a dangling bond as shown in Fig. 2a and b. Lastly, we discuss adsorptions of Si atoms as well as F- and Br-chemistries and demonstrate their similarities and differences in terms of reactivity and thermodynamics.
Figure 1. Top view and side view of a) CH$_3$(ads), b) CH$_2$(ads) and c) C$_2$H$_4$(ads) pre-deposited on the Si face of the Si$_{19}$C$_{19}$ cluster.
Figure 2. Top view and side view of a) H(ads) and b) *(ads) pre-deposited on the C face of the Si_{19}C_{19} cluster.

Computational Methods

The surface of 4H-SiC is modeled using Si_{19}C_{19} and Si_{24}C_{24} clusters. The central surface sites (two on Si_{19}C_{19} and three on Si_{24}C_{24}) are chosen for the study. Si_{19}C_{19} is used in the calculations of adsorption and the first step of cluster formation, while Si_{24}C_{24} is employed in the second step of cluster formation. To preserve the SiC bulk geometry, both clusters are terminated at the edges by hydrogen atoms. Adsorptions are studied on both the Si face and the C face of the cluster. On the Si face, we consider three adsorption sites: CH_{3}(ads), CH_{2}(ads) and C_{2}H_{4}(ads) as shown in
Fig. 1a – 1c, while on the C face, two adsorption sites, H(ads) and *(ads), are selected as shown in Fig. 2a and b. In this study, *(ads) refers to a surface site terminated by a dangling bond.

All ground state and transition state (TS) structures are optimized using the density functional theory (DFT) with the B3LYP functional \(^{13,14}\) and the LanL2DZ basis set \(^{15,16}\) together with the D3 dispersion corrections from Grimme et al. \(^{17}\). Harmonic frequency calculations are performed at the same level of theory on the optimized structures. B3LYP electronic energies are replaced with the energy calculated using the M06-2X functional \(^{18}\) and Dunning’s basis set cc-pVTZ \(^{19}\). The transition state (TS) structures are verified by visualizing the vibrational displacement associated with the imaginary frequencies. Zero point energy correction is applied to all energies in the study. All quantum chemical calculations are performed using the Gaussian 09 software \(^{20}\).

The energies and Gibbs free energies of reaction are derived using

\[
\Delta_R E^o = \left( \sum E^o_{products} \right) - \left( \sum E^o_{reactants} \right), \tag{1}
\]

\[
\Delta_R G^o = \left( \sum G^o_{products} \right) - \left( \sum G^o_{reactants} \right). \tag{2}
\]

The energies and Gibbs free energies of activation are derived using

\[
\Delta_{TS} E^o = \left( \sum E^o_{TS} \right) - \left( \sum E^o_{reactants} \right), \tag{3}
\]

\[
\Delta_{TS} G^o = \left( \sum G^o_{TS} \right) - \left( \sum G^o_{reactants} \right). \tag{4}
\]

\(E^o_{reactants}, E^o_{products}, E^o_{TS}\) refer to the energies of the reactants, products and transition states, respectively. For a reaction involving gas phase species, the ground state energy is defined with respect to the asymptote condition where the surface and the gas are separated at infinite distance.
This is not to be confused with the physisorbed state, which is known to be unstable at high temperature.

**Reaction Rates.** The conventional transition state theory (TST) is applied to calculate the rate constant. This implies that rapid equilibrium is assumed between the reactants and activation complex. TST is applicable when a tight transition state exists between the reactant and product states. Similar to our previous study, we use the modified rate equations from Reuter and Scheffler’s work.

**Adsorption.** Adsorption rate \((R_{ads})\) of a reaction in the form, \(A(g) + B(ads) \rightarrow \text{product}(ads)\), is obtained as follows.

\[
R_{ads} = A_s f_{ads} \exp\left(-\Delta_{TS}E^\circ/k_B T\right) \cdot \Phi_A \cdot \Theta_B, \quad (5)
\]

Here the adsorption rate \(R_{ads}\) is in the unit of molecule sites\(^{-1}\) s\(^{-1}\). \(A_s\) is the surface area per site of surface species B, assumed equal to the area per one lattice site on the Si face and the C face of 4H–SiC, 8.178x10\(^{-20}\) m\(^2\) as derived using the lattice constant of 3.073 Å\(^2\). \(\Delta_{TS}E^\circ\) is the activation energy of adsorption at 0 K. \(k_B\) and \(T\) refer to the Boltzmann constant and the process temperature, respectively. \(\Theta_B\) is the surface fraction of B(ads), and \(\Phi_A\) is the impingement rate of species A calculated using

\[
\Phi_A = \gamma_A p / \sqrt{2\pi m_A k_B T}. \quad (6)
\]

\(\gamma_A,\ p\) and \(m_A\) refer respectively to the mole fraction of gaseous species A, the total pressure and the mass of gaseous species A. The factor \(f_{ads}\) in Eq. 5 is a factor derived from the partition functions,
\[ f_{\text{ads}} = q_{\text{vib,el}}^{TS} / \left( q_{2D-\text{Trans}}^{\text{gas}} \cdot q_{\text{int}}^{\text{gas}} \cdot q_{\text{surf}}^{\text{surf}} \right). \] (7)

Here the partition function of a surface species contains only the vibrational and electronic parts, with the translational and rotational parts discarded. This applies to \( q^{TS} \) of the transition state and \( q^{\text{surf}} \) of a surface species, B(ads). The partition of the gas, \( q^{\text{gas}} \), includes all degrees of freedom except the translation along the reaction coordinate. In Eq. 7, \( q^{\text{gas}} \) is divided into two parts. The \( q^{\text{gas}}_{\text{int}} \) contains the vibrational, rotational and electronic parts, while \( q^{\text{gas}}_{2D-\text{Trans}} \) is the 2-dimensional, translational part of the partition function calculated using \( q^{\text{gas}}_{2D-\text{Trans}} = A_s \cdot 2 \pi m_A k_B T / h^2 \). Here we assume that the gaseous species that strike on the surface site must reside within the area \( A_s \).

All partition functions are extracted from the Gaussian 09 calculations. \(^2\)

The sticking coefficient \((S_A)\), which is defined as the probability (from 0 to 1) that the gaseous species A will stick on the surface per strike, is calculated using \( S_A = R_{\text{ads}} / (A_s \cdot \Phi_A \cdot \Theta_B) \). From Eq. 5−7, we obtain

\[ S_A = f_{\text{ads}} \exp(-\Delta_{TS}E^\circ / k_B T). \] (8)

**Desorption.** Desorption rate \((R_{de})\) of a reaction in the form, \( A(\text{ads}) \rightarrow \text{product(s)}, \) is obtained using

\[ R_{de} = f_{de} \left( \frac{k_B T}{h} \right) \exp(-\Delta_{TS}E^\circ / k_B T) \cdot \Theta_A. \] (9)

\( \Delta_{TS}E^\circ \) is the activation energy of desorption at 0 K. \( \Theta_A \) is the fraction of surface occupied by A(ads). \( f_{de} \) is the factor derived from the partition functions,

\[ f_{de} = q_{\text{vib,el}}^{TS} / q_{\text{vib,el}}^{\text{ads}}. \] (10)
where $q^{TS}$ and $q^{ads}$ are the partition functions of the transition state and the adsorbed species, $A(ads)$.

**On-surface Reaction.** Reaction rate of an on-surface reaction in the form, $A(ads) + B(ads) \rightarrow \text{product(s)}$, is obtained using

$$R_{on-surf} = f_{on-surf} \left( \frac{k_B T}{h} \right) \exp \left( -\frac{\Delta_{TS}E^o}{k_B T} \right) \Theta_{AB}. \quad (11)$$

$\Delta_{TS}E^o$ is the activation energy of the on-surface reaction at 0 K. $\Theta_{AB}$ is the surface fraction of a pair of $A(ads) + B(ads)$. $f_{on-surf}$ is the factor derived from the partition functions,

$$f_{on-surf} = \frac{q^{TS}_{vib,el}}{q^{surf}_{vib,el}}. \quad (12)$$

where $q^{TS}$ and $q^{surf}$ are the partition functions of the transition state and the pair of $A(ads) + B(ads)$.

**Results and Discussion**

This section is divided into three parts. The first and second parts are focused on the adsorptions of SiH, SiH$_2$, SiCl, SiHCl and SiCl$_2$ and their subsequent surface reactions on the Si face and on the C face of 4H-SiC. The last subsection is focused on the adsorptions of Si atoms and of SiX, SiHX and SiX$_2$ for X being F and Br, which leads to the discussion of the similarities and dissimilarities between the different CVD chemistries.

**1 Adsorptions and surface reactions on the Si face of 4H-SiC.**
1.1 Adsorptions. We consider three types of adsorption sites on the Si face: CH$_3$(ads), CH$_2$(ads) and C$_2$H$_4$(ads), which are the products of surface reactions of CH$_3$, C$_2$H$_4$ and C$_2$H$_2$ gases as reported in our previous work $^{12}$.

Adsorptions on CH$_3$(ads) of SiH, SiH$_2$, SiCl, SiHCl, and SiCl$_2$ gases occur by breaking a C-H bond in CH$_3$(ads) and forming a new C-Si bond and Si-H bond. Fig. 3a and b show the transition state and the product of SiH adsorption on CH$_3$(ads). Adsorptions of SiH, SiH$_2$, SiCl, SiHCl, and SiCl$_2$ gases all produce large energy barriers ($\Delta_T$G°) and positive changes in the Gibbs free energies, $\Delta_R$G°, at 1600 °C which is the temperature typically used in SiC CVD process. Large energy barriers ($\Delta_T$G°) lead to very low sticking coefficients for all species, as shown for R1 – R5 in Table 1. The positive $\Delta_R$G° indicate that desorption, i.e. the reverse of the adsorption reaction, is thermodynamically more favorable and that desorption rates are faster than adsorption rates, as shown in Table 2.

The reactivity of CH$_3$(ads) can be enhanced, for example by abstraction of an H atom

$$\text{CH}_3(\text{ads}) + \text{H(g)} \rightarrow \text{CH}_2(\text{ads}) + \text{H}_2(\text{g}), \quad (R16)$$

which occurs with $\Delta_R$G° and $\Delta_T$G° of -82 and 248 kJ/mol at 1600 °C $^{12}$. The H-abstraction process R16 creates a dangling bond on the C site and thereby increasing its reactivity. As a result, adsorptions of Si species on CH$_2$(ads) are more favorable than on CH$_3$(ads) as shown in R6 – R10 in Table 1. In addition, adsorptions of Si species on CH$_2$(ads) also occur without the presence of transition states. However, their $\Delta_R$G° are positive, meaning that desorptions are again more favorable and occur with faster rates, as shown in Table 2.
Now let us move on to adsorptions of Si species on a C$_2$H$_4$(ads) molecule. A C$_2$H$_4$(ads) molecule is a product of C$_2$H$_2$ adsorption and its subsequent reactions. Similar to CH$_3$(ads), the C$_2$H$_4$(ads) molecule has no surface dangling bond. Thus, adsorptions on C$_2$H$_4$(ads) species require breaking of the C-C bond in the molecule before new Si-C bonds can be formed. Figure 4a and b show the transition state and the product of SiH adsorption on a C$_2$H$_4$(ads) molecule. Similar to the adsorptions on CH$_3$(ads), adsorptions of Si species on C$_2$H$_4$(ads) species create large energy barriers ($\Delta_{TS}G^\circ$) at 1600 °C. It should be noted that despite $\Delta_RTG^\circ$ being negative in some cases, all transition barriers $\Delta_{TS}G^\circ$ are significantly larger than the other adsorption sites considered previously. This is likely due to the species itself being more stable. As a result, the sticking coefficients of the Si species are the lowest on C$_2$H$_4$(ads) species. C$_2$H$_4$(ads) species is thus the least active adsorption site considered here. In addition, their large transition barriers also make it hard for desorptions to occur via the direct reverse of R11 – R15. The formation of two Si-C bonds thus helps stabilizing the surface species.

Similar to CH$_3$(ads), the reactivity of C$_2$H$_4$(ads) species can be enhanced by interacting with a hydrogen atom,

$$\text{C}_2\text{H}_4(\text{ads}) + \text{H}(g) \rightarrow \text{CH}_2(\text{ads}) + \text{CH}_3(\text{ads}), \quad (\text{R17})$$

which occurs with $\Delta_RTG^\circ$ and $\Delta_{TS}G^\circ$ of 1 and 295 kJ/mol at 1600 °C, as shown in Table 1. Reaction R17 breaks the C-C bond within the species and creates a dangling bond on one of the C atoms. Adsorptions of Si species on the newly created CH$_2$(ads) occur without the presence of a transition state and their products are accompanied by an adjacent CH$_3$(ads).

In conclusion, from the sticking coefficients listed in Table 1, we find that the adsorption processes with the largest sticking coefficients ($S$) are as follows: adsorption of SiH on CH$_3$(ads) ($S =$
adsorption of SiCl on CH₃(ads) (S = 4 × 10⁻⁵), adsorption of SiH₂ on CH₃(ads) (S = 3 × 10⁻⁵) and adsorption of SiH on C₂H₄(ads) species (S = 9 × 10⁻⁶). The growth rate $V_H$ associated with each adsorption can be obtained using $V_H = R_{ads} \cdot h_{ML}$, with $h_{ML}$ being the height of one SiC bilayer, ~2.5131x10⁻¹⁰ m. We assume $\Theta$ of 1.0 for both CH₃(ads) and C₂H₄(ads) species which are their maximum values. The molar fractions, $\Phi$, of the Si-species were taken from thermodynamic equilibrium calculations at 1600 °C ($\Phi \sim 10^{-5}$ for SiH and SiH₂, $\Phi \sim 10^{-3}$ for SiCl and SiCl₂ and $\Phi \sim 10^{-4}$ for SiHCl). We obtain the following growth rates: ~0.25 µm/hour for SiCl on CH₃(ads), ~0.08 µm/hour for SiCl on C₂H₄(ads) species, ~0.03 µm/hour for SiH on CH₃(ads) and ~0.002 µm/hour for SiH₂ on CH₃(ads). These growth rates are much too low to contribute significantly to the growth rate observed experimentally, ~100 µm/hour. Instead, we may speculate that adsorptions occur more efficiently on CH₂(ads) from their much smaller $\Delta_R G^\circ$ and lacking of transition states. By assuming the sticking coefficients of the Si species to be 1.0 on CH₂(ads) and using $\Theta$ equal to 1.0 together with the same molar fractions of the Si species as before, we obtain the growth rates of 84 µm/hour for SiH, 82 µm/hour for SiH₂, ~6×10³ µm/hour for SiCl and SiHCl, and ~455 µm/hour for SiCl₂. These growth rates are much larger than the experimental value because we have assumed $\Theta$ of CH₂(ads) equal to 1.0, which is the maximum value possible, and we have so far neglected the effects of desorptions. In fact, with their $\Delta_R G^\circ$ being positive, adsorptions on CH₂(ads) are expected to occur with the rates which are significantly smaller than their desorptions.

**Table 1** The energies (0 K), standard Gibbs free energies (1600 °C) and sticking coefficients of SiH, SiH₂, SiCl, SiHCl and SiCl₂ on CH₃(ads), CH₂(ads) and C₂H₄(ads) species pre-deposited on the Si face of 4H–SiC. The (free) energies are presented in the unit of kJ/mol, calculated with respect to the energy of the reactant state at asymptote condition.
### Adsorptions on CH₃(ads)

<table>
<thead>
<tr>
<th>Rate &amp; Reaction</th>
<th>∆ₚE°</th>
<th>∆ₚG°</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1 SiH(g) + CH₃(ads) → SiH₂-CH₂(ads)</td>
<td>-157</td>
<td>94</td>
<td>3 × 10⁻⁴</td>
</tr>
<tr>
<td>R2 SiH₂(g) + CH₃(ads) → SiH₃-CH₂(ads)</td>
<td>-203</td>
<td>91</td>
<td>3 × 10⁻⁵</td>
</tr>
<tr>
<td>R3 SiCl(g) + CH₃(ads) → SiHCl-CH₂(ads)</td>
<td>-124</td>
<td>146</td>
<td>4 × 10⁻⁵</td>
</tr>
<tr>
<td>R4 SiHCl(g) + CH₃(ads) → SiH₂Cl-CH₂(ads)</td>
<td>-185</td>
<td>132</td>
<td>7 × 10⁻⁷</td>
</tr>
<tr>
<td>R5 SiCl₂(g) + CH₃(ads) → SiHCl₂-CH₂(ads)</td>
<td>-134</td>
<td>177</td>
<td>492 8 × 10⁻⁹</td>
</tr>
</tbody>
</table>

### Adsorptions on CH₂(ads)

<table>
<thead>
<tr>
<th>Rate &amp; Reaction</th>
<th>∆ₚE°</th>
<th>∆ₚG°</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>R6 SiH(g) + CH₂(ads) → SiH-CH₂(ads)</td>
<td>-320</td>
<td>15</td>
<td>-</td>
</tr>
<tr>
<td>R7 SiH₂(g) + CH₂(ads) → SiH₂-CH₂(ads)</td>
<td>-247</td>
<td>65</td>
<td>-</td>
</tr>
<tr>
<td>R8 SiCl(g) + CH₂(ads) → SiCl-CH₂(ads)</td>
<td>-306</td>
<td>37</td>
<td>-</td>
</tr>
<tr>
<td>R9 SiHCl(g) + CH₂(ads) → SiHCl-CH₂(ads)</td>
<td>-226</td>
<td>113</td>
<td>-</td>
</tr>
<tr>
<td>R10 SiCl₂(g) + CH₂(ads) → SiCl₂-CH₂(ads)</td>
<td>-183</td>
<td>128</td>
<td>-</td>
</tr>
</tbody>
</table>

### Adsorptions on C₂H₄(ads)

<table>
<thead>
<tr>
<th>Rate &amp; Reaction</th>
<th>∆ₚE°</th>
<th>∆ₚG°</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>R11 SiH(g) + C₂H₄(ads) → SiH-(CH₂)₂(ads)</td>
<td>-275</td>
<td>140</td>
<td>-1</td>
</tr>
<tr>
<td>R12 SiH₂(g) + C₂H₄(ads) → SiH₂-(CH₂)₂(ads)</td>
<td>-327</td>
<td>206</td>
<td>-28</td>
</tr>
<tr>
<td>R13 SiCl(g) + C₂H₄(ads) → SiCl-(CH₂)₂(ads)</td>
<td>-245</td>
<td>148</td>
<td>36</td>
</tr>
<tr>
<td>R14 SiHCl(g) + C₂H₄(ads) → SiHCl-(CH₂)₂(ads)</td>
<td>-312</td>
<td>234</td>
<td>7</td>
</tr>
<tr>
<td>R15 SiCl₂(g) + C₂H₄(ads) → SiCl₂-(CH₂)₂(ads)</td>
<td>-273</td>
<td>275</td>
<td>50</td>
</tr>
</tbody>
</table>

### Hydrogen abstraction

<table>
<thead>
<tr>
<th>Rate &amp; Reaction</th>
<th>∆ₚE°</th>
<th>∆ₚG°</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>R16 CH₃(ads) + H(g) → CH₂(ads) + H₂(ads)</td>
<td>-25</td>
<td>52 a)</td>
<td>-82 a)</td>
</tr>
<tr>
<td>R17 C₂H₄(ads) + H(g) → CH₂(ads) + CH₃(ads)</td>
<td>-138</td>
<td>96</td>
<td>1</td>
</tr>
</tbody>
</table>

a) Ref. 12.

Table 2 The adsorption and desorption rate constants at 1600 °C of SiH, SiH₂, SiCl, SiHCl and SiCl₂ on CH₃(ads) and C₂H₄(ads) pre-deposited on the Si face of 4H–SiC.
<table>
<thead>
<tr>
<th>Adsorptions on CH(_3)(ads)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R1  SiH(g) + CH(_3)(ads) → SiH(_2)-CH(_2)(ads)</td>
<td>3 \times 10^{-1}</td>
<td>1 \times 10^7</td>
</tr>
<tr>
<td>R2  SiH(_2)(g) + CH(_3)(ads) → SiH(_3)-CH(_2)(ads)</td>
<td>2 \times 10^{-2}</td>
<td>1 \times 10^6</td>
</tr>
<tr>
<td>R3  SiCl(g) + CH(_3)(ads) → SiHCl-CH(_2)(ads)</td>
<td>3 \times 10^{-2}</td>
<td>5 \times 10^7</td>
</tr>
<tr>
<td>R4  SiHCl(g) + CH(_3)(ads) → SiH(_2)Cl-CH(_2)(ads)</td>
<td>4 \times 10^{-4}</td>
<td>3 \times 10^5</td>
</tr>
<tr>
<td>R5  SiCl(_2)(g) + CH(_3)(ads) → SiHCl(_2)-CH(_2)(ads)</td>
<td>4 \times 10^{-6}</td>
<td>6 \times 10^4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Adsorptions on C(_2)H(_4)(ads)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>R11 SiH(g) + C(_2)H(_4)(ads) → SiH-(CH(_2))(_2)(ads)</td>
<td>2 \times 10^{-2}</td>
<td>5 \times 10^2</td>
</tr>
<tr>
<td>R12 SiH(_2)(g) + C(_2)H(_4)(ads) → SiH(_2)-(CH(_2))(_2)(ads)</td>
<td>9 \times 10^{-5}</td>
<td>9 \times 10^{-1}</td>
</tr>
<tr>
<td>R13 SiCl(g) + C(_2)H(_4)(ads) → SiCl-(CH(_2))(_2)(ads)</td>
<td>8 \times 10^{-3}</td>
<td>6 \times 10^3</td>
</tr>
<tr>
<td>R14 SiHCl(g) + C(_2)H(_4)(ads) → SiHCl-(CH(_2))(_2)(ads)</td>
<td>2 \times 10^{-6}</td>
<td>2 \times 10^{-1}</td>
</tr>
<tr>
<td>R15 SiCl(_2)(g) + C(_2)H(_4)(ads) → SiCl(_2)-(CH(_2))(_2)(ads)</td>
<td>2 \times 10^{-7}</td>
<td>4 \times 10^{-1}</td>
</tr>
</tbody>
</table>

\(R_{ads}/p\gamma_g\Theta_s\), are calculated using Eq. 5-8. Here, the adsorption rate \(R_{ads}\) is in molecule per site per second. The total pressure \((p)\) is in Pascal. The gaseous molar fraction \((\gamma_g)\) and the surface fraction \((\Theta_s)\) are unitless. The surface area per site of CH\(_3\)(ads) is assumed equal to 8.178\(\times\)10\(^{-20}\) m\(^2\) which is the area per one lattice site on the Si-face of 4H–SiC. The area per site of C\(_2\)H\(_4\)(ads) is assumed equal to 1.636\(\times\)10\(^{-19}\) m\(^2\) which is the area per two lattice sites.

\(R_{de}/\Theta_s\), are calculated using Eq. 9-10. Here, the desorption rate \(R_{de}\) is in molecule per site per second. The surface fraction \((\Theta_s)\) is unitless.
Figure 3. Top view and side view of a) the transition state and b) the product of SiH adsorption on CH$_3$(ads).
1.2. Cluster formations. In the previous subsection, we showed that based on the rate derived it is unlikely for adsorptions on CH$_3$(ads) and on C$_2$H$_4$(ads) species to contribute significantly to the growth. It could be that the main adsorption route occurs mainly via CH$_2$(ads). We also show that adsorptions on CH$_3$(ads), C$_2$H$_4$(ads) and CH$_2$(ads) all occur with positive $\Delta_R G^\circ$. Thus, for all processes considered, desorptions are more favorable than adsorptions. In order for the growth to proceed in the forward direction, it is thus necessary that there are subsequent reaction path(s)
following adsorptions which helps reducing the total $\Delta R G^\circ$ and stabilizing the final products. In addition, this path(s) should occur with a rate that is fast enough, at least comparable to that of the desorption rate. We propose that one route for this is by formation of larger surface species, or a cluster.

In the first step following adsorptions, let us consider a bonding process between the adsorbed species and an adjacent CH$_3$(ads), as shown in R18-R22 in Table 3. In Figure 5a-c, we show an example of SiH-CH$_2$(ads), which is the product of SiH adsorption on CH$_2$(ads), forming a bond with its adjacent CH$_3$(ads). This process occurs by breaking a C-H bond in CH$_3$(ads) and forming new C-Si and Si-H bonds. As shown in Table 3, the processes R18-R22 are thermodynamically preferable with negative $\Delta R G^\circ$ at 1600 °C. In addition, their transition barriers are relatively small, especially for the interactions R18 and R20, resulting in the forward rate constants as high as $10^9$ molecule site$^{-1}$ second$^{-1}$ as shown in Table 4. These rates are fast enough to compete with desorption processes. From the rate constants shown in Table 4, it should be noted that R19, R20 and R22 which are the subsequent reactions following the adsorptions of SiH$_2$, SiHCl and SiCl$_2$, are ~100-1000 times slower than R18 and R20 which are the subsequent reactions following the adsorptions of SiH and SiCl. This together with the fact that $\Delta R G^\circ$ of SiH$_2$, SiHCl and SiCl$_2$ adsorptions are much more positive than $\Delta R G^\circ$ of SiH and SiCl adsorptions implies that the growth contributions from SiH$_2$, SiHCl and SiCl$_2$ are likely much less than from SiH and SiCl.

Following this step, the surface species can be stabilized further by forming another Si-C bond with another CH$_3$(ads) via R23-R26 shown in Table 3. An example of an interaction between SiH$_2$-(CH$_2$)$_2$(ads) and an adjacent CH$_3$(ads), which is the reaction following R18, is shown in Fig. 6a-c. Via these two steps, SiC growth via SiH adsorption may proceed as follows,
SiH(g) + CH₂(ads) → SiH-CH₂(ads), (R6)

SiH-CH₂(ads) + CH₃(ads) → SiH₂-(CH₂)₂(ads), (R18)

and SiH₂-(CH₂)₂(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + H₂(g).

(R23)

These steps produce SiH-(CH₂)₃(ads) as the final product and produces a total change in $\Delta R G°$ of -366 kJ/mol at 1600 °C. The step-by-step change in the Gibbs free energy is depicted in Fig 7.

Similarly, SiH₂ adsorption and subsequent reactions are as follows

SiH₂(g) + CH₂(ads) → SiH₂-CH₂(ads), (R7)

SiH₂-CH₂(ads) + CH₃(ads) → SiH₂-(CH₂)₂(ads) + H(g), (R19)

and

SiH₂-(CH₂)₂(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + H₂(g).

(R23)

This leads to the production of SiH-(CH₂)₃(ads) with a total change in $\Delta R G°$ of -238 kJ/mol at 1600 °C.

SiCl adsorption and subsequent reactions may occur via two different routes, as shown in Fig. 8.

SiCl(g) + CH₂(ads) → SiCl-CH₂(ads), (R8)

SiCl-CH₂(ads) + CH₃(ads) → SiHCl-(CH₂)₂(ads), (R20)

and
SiHCl-(CH₂)₂(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + HCl(g), \hspace{1cm} (R24)

or

SiHCl-(CH₂)₂(ads) + CH₃(ads) → SiCl-(CH₂)₃(ads) + H₂(g). \hspace{1cm} (R25)

The product SiH-(CH₂)₃(ads) occurs via the combination of R8, R20 and R24 with a total change in $\Delta R G°$ of -260 kJ/mol at 1600 °C, while the product SiCl-(CH₂)₃(ads) occurs by replacing R24 with R25 and produces a total change in $\Delta R G°$ of -318 kJ/mol at 1600 °C. It should be noted that $\Delta T S G°$ of R24 and R25 are relatively similar (269 and 289 kJ/mol). Thus, the two processes are highly competitive to each other.

SiHCl adsorption and subsequent reactions occurs as follows,

SiHCl(g) + CH₂(ads) → SiHCl-CH₂(ads), \hspace{1cm} (R9)

SiHCl-CH₂(ads) + CH₃(ads) → SiHCl-(CH₂)₂(ads) + H(g), \hspace{1cm} (R21)

and

SiHCl-(CH₂)₂(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + HCl(g), \hspace{1cm} (R24)

or

SiHCl-(CH₂)₂(ads) + CH₃(ads) → SiCl-(CH₂)₃(ads) + H₂(g). \hspace{1cm} (R25)
The product SiH-(CH₂)₃(ads) occurs via the combination of R9, R21 and R24 with a total change of -138 kJ/mol in $\Delta_R G^\circ$ at 1600 °C, while the product SiCl-(CH₂)₃(ads) occurs by replacing R24 with R25 producing a total change in $\Delta_R G^\circ$ of -196 kJ/mol at 1600 °C.

Adsorption of SiCl₂ and its subsequent reactions produce SiCl-(CH₂)₃(ads) with the change in $\Delta_R G^\circ$ of -139 kJ/mol at 1600 °C. This happens via

$$\text{SiCl}_2(g) + \text{CH}_2(\text{ads}) \rightarrow \text{SiCl}_2\text{-CH}_2(\text{ads}), \quad (\text{R}10)$$

$$\text{SiCl}_2\text{-CH}_2(\text{ads}) + \text{CH}_3(\text{ads}) \rightarrow \text{SiCl}_2\text{-(CH}_2)_2(\text{ads}) + \text{H}(g), \quad (\text{R}22)$$

and

$$\text{SiCl}_2\text{-(CH}_2)_2(\text{ads}) + \text{CH}_3(\text{ads}) \rightarrow \text{SiCl}-(\text{CH}_2)_3(\text{ads}) + \text{HCl}(g). \quad (\text{R}26)$$

Let us now consider reactions R27 and R28,

$$\text{SiH}-(\text{CH}_2)_3(\text{ads}) + \text{H}(g) \rightarrow \text{Si}^*-(\text{CH}_2)_3(\text{ads}) + \text{H}_2(g), \quad (\text{R}27)$$

and

$$\text{SiCl}-(\text{CH}_2)_3(\text{ads}) + \text{H}(g) \rightarrow \text{Si}^*-(\text{CH}_2)_3(\text{ads}) + \text{HCl}(g), \quad (\text{R}28)$$

which help creating a surface dangling bond, Si*- (CH₂)₃(ads), which was shown to be important for hydrocarbon adsorptions for the next layer ¹². As shown in Table 3 and 4, it is more difficult to remove Cl-termination in comparison to H-termination. Nevertheless, as the CVD process condition is known to produce a significant amount of H atoms in the gas phase ²⁵, the rates of R27 and R28 likely occur much faster than adsorptions.
**Table 3** The energies (0 K) and standard Gibbs free energies (1600 °C) of the clustering process.

The (free) energies are presented in the unit of kJ/mol.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Equations</th>
<th>$\Delta_R E^\circ$</th>
<th>$\Delta_{TS} E^\circ$</th>
<th>$\Delta_R G^\circ$</th>
<th>$\Delta_{TS} G^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st step of cluster formation process</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R18</td>
<td>SiH-CH$_2$(ads) + CH$_3$(ads) → SiH$_2$-(CH$_2$)$_2$(ads)</td>
<td>-219</td>
<td>95</td>
<td>-158</td>
<td>151</td>
</tr>
<tr>
<td>R19</td>
<td>SiH$_2$-CH$_2$(ads) + CH$_3$(ads) → SiH$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>57</td>
<td>177</td>
<td>-80</td>
<td>246</td>
</tr>
<tr>
<td>R20</td>
<td>SiCl-CH$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads)</td>
<td>-182</td>
<td>142</td>
<td>-140</td>
<td>176</td>
</tr>
<tr>
<td>R21</td>
<td>SiHCl-CH$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads) + H(g)</td>
<td>46</td>
<td>167</td>
<td>-94</td>
<td>235</td>
</tr>
<tr>
<td>R22</td>
<td>SiCl$_2$-CH$_2$(ads) + CH$_3$(ads) → SiCl$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>43</td>
<td>189</td>
<td>-100</td>
<td>228</td>
</tr>
<tr>
<td>2nd step of cluster formation process</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R23</td>
<td>SiH$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiH-(CH$_2$)$_3$(ads) + H$_2$(g)</td>
<td>-34</td>
<td>292</td>
<td>-223</td>
<td>309</td>
</tr>
<tr>
<td>R24</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiH-(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>59</td>
<td>231</td>
<td>-157</td>
<td>269</td>
</tr>
<tr>
<td>R25</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiCl-(CH$_2$)$_3$(ads) + H$_2$(g)</td>
<td>-44</td>
<td>266</td>
<td>-215</td>
<td>289</td>
</tr>
<tr>
<td>R26</td>
<td>SiCl$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiCl-(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>37</td>
<td>243</td>
<td>-167</td>
<td>288</td>
</tr>
<tr>
<td>Surface dangling bond creation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R27</td>
<td>SiH-(CH$_2$)$_3$(ads) + H(g) → Si*--(CH$_2$)$_3$(ads) + H$_2$(g)</td>
<td>-63</td>
<td>12</td>
<td>-77</td>
<td>181</td>
</tr>
<tr>
<td>R28</td>
<td>SiCl-(CH$_2$)$_3$(ads) + H(g) → Si*--(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>40</td>
<td>90</td>
<td>-19</td>
<td>258</td>
</tr>
</tbody>
</table>

**Table 4** The forward and reverse rate constants of subsequent reactions at 1600 °C in the unit of molecule per site per second.
### 1st step of cluster formation process

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward rate constants</th>
<th>Reverse rate constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>R18: SiH-CH₂(ads) + CH₃(ads) → SiH₂-(CH₂)₂(ads)</td>
<td>2 × 10⁹ a)</td>
<td>9 × 10⁴ a)</td>
</tr>
<tr>
<td>R19: SiH₂-CH₂(ads) + CH₃(ads) → SiH₂-(CH₂)₂(ads) + H(g)</td>
<td>5 × 10⁶ a)</td>
<td>6 × 10⁻¹ b)</td>
</tr>
<tr>
<td>R20: SiCl-CH₂(ads) + CH₃(ads) → SiHCl-(CH₂)₂(ads)</td>
<td>5 × 10⁸ a)</td>
<td>6 × 10⁴ a)</td>
</tr>
<tr>
<td>R21: SiHCl-CH₂(ads) + CH₃(ads) → SiHCl-(CH₂)₂(ads) + H(g)</td>
<td>1 × 10⁷ a)</td>
<td>5 × 10⁻¹ b)</td>
</tr>
</tbody>
</table>

### 2nd step of cluster formation process

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward rate constants</th>
<th>Reverse rate constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>R23: SiH₂-(CH₂)₂(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + H₂(g)</td>
<td>1 × 10⁵ a)</td>
<td>2 × 10⁻⁶ b)</td>
</tr>
<tr>
<td>R24: SiHCl-(CH₂)₃(ads) + CH₃(ads) → SiH-(CH₂)₃(ads) + HCl(g)</td>
<td>1 × 10⁶ a)</td>
<td>1 × 10⁻³ b)</td>
</tr>
<tr>
<td>R25: SiHCl-(CH₂)₃(ads) + CH₃(ads) → SiCl-(CH₂)₃(ads) + H₂(g)</td>
<td>3 × 10⁵ a)</td>
<td>3 × 10⁻⁶ b)</td>
</tr>
<tr>
<td>R26: SiCl₂-(CH₂)₂(ads) + CH₃(ads) → SiCl-(CH₂)₃(ads) + HCl(g)</td>
<td>4 × 10⁵ a)</td>
<td>6 × 10⁻⁵ b)</td>
</tr>
</tbody>
</table>

### Surface dangling bond creation

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward rate constants</th>
<th>Reverse rate constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>R27: SiH-(CH₂)₃(ads) + H(g) → Si*- (CH₂)₃(ads) + H₂(g)</td>
<td>3 × 10⁴ b)</td>
<td>7 × 10¹ b)</td>
</tr>
<tr>
<td>R28: SiCl-(CH₂)₃(ads) + H(g) → Si*- (CH₂)₃(ads) + HCl(g)</td>
<td>7 × 10¹ b)</td>
<td>2 × 10¹ b)</td>
</tr>
</tbody>
</table>

---

a) Calculated using Eq. 9-10. The rate constant is defined as \( R / \Theta_s \) where \( R \) is the reaction rate in molecule per site per second and \( \Theta_s \) is the surface fraction which is unitless.

b) Calculated using Eq. 5-8. The rate constant is defined as \( R / p \gamma_g \Theta_s \) where the reaction rate \( (R) \) is in molecule per site per second, the total pressure \( (p) \) is in pascal, and the gaseous molar fraction \( (\gamma_g) \) and the surface fraction \( (\Theta_s) \) are unitless. The surface area per site of SiHₙXₘ-CH₂(ads) is assumed equal to 8.178x10⁻²⁰ m² which is the area per one lattice site on the Si-face of 4H–SiC.
The areas per site of SiH_nX_m-(CH_2)_2(ads) and SiX-(CH_2)_3(ads) are assumed equal to 1.636x10^{-19} and 2.453x10^{-19} m^2 respectively, which are the areas per two and three lattice sites on the Si-face of 4H–SiC.

![Diagram](image)
**Figure 5** Top view and side view of a) the reactants, b) the transition state, and b) the product of 1st step of cluster formation between SiH-CH$_2$(ads) and an adjacent CH$_3$(ads).
Figure 6 Top view and side view of a) the reactants, b) the transition state, and b) the product of 2nd step of cluster formation between SiH$_2$-(CH$_2$)$_2$(ads) and an adjacent CH$_3$(ads).
Figure 7 Reaction scheme of SiC growth from SiH(g) adsorption and cluster formation
**Figure 8** Reaction scheme of SiC growth from SiCl(g) adsorption and cluster formation.
2 Adsorptions on the C face of 4H-SiC. Here we consider two types of surface sites: H(ads) and *(ads), which refer respectively to a surface site on the C face terminated by an H atom and by a dangling bond. Adsorptions of the Si-species on H(ads) occurs by breaking a C-H bond and forming a Si-H bond and a Si-C bond as shown in Fig. 9a and b. The processes are present with large energy barriers ($\Delta T S G^\circ$) together with large positive $\Delta R G^\circ$ as shown in Table 5. This results in low sticking coefficients for all adsorbing species. As shown in Table 5, the sticking coefficients on H(ads) from largest to smallest are SiH > SiCl > SiH$_2$ $\gg$ SiHCl $\gg$ SiCl$_2$. With the growth rate $V_H$ obtained using $V_H = R_{ads} \cdot h_M L$, with $h_M L$ being 2.5131x10$^{-10}$ m, and using $\Theta$ equal to 1.0 together with the same molar fractions of the Si species similar to section 1.1, we obtain the adsorption rates (from highest to lowest) to be $\sim$1.1 µm/hour for SiCl; $\sim$0.2 µm/hour for SiH; $\sim$0.005 µm/hour for SiH$_2$; and smaller for the rest. These rates are again too low to contribute to the growth rate observed experimentally.

Adsorptions of the Si-species on *(ads), on the other hand, occurs with much smaller $\Delta R G^\circ$ and without transition states due to the presence of the surface dangling bond. *(ads) can be created from H(ads) via an interaction with a hydrogen atom,

\[ H(ads) + H(g) \rightarrow *(ads) + H_2(g), \]  

which occurs with $\Delta R G^\circ$ and $\Delta T S G^\circ$ of -46 and 211 kJ/mol at 1600 °C. Unlike adsorptions on the Si face, adsorptions of SiH, SiH$_2$ and SiCl on *(ads) occur with negative $\Delta R G^\circ$ at 1600 °C, as shown in Table 5. This indicates that the adsorbed species on the surface are stable without any help from subsequent reactions. From $\Delta R G^\circ$, we might expect the following trend of the adsorption rates (from largest to smallest): SiH > SiCl > SiH$_2$ $\gg$ SiHCl $\gg$ SiCl$_2$, which is the same order as above for H(ads). Since adsorptions on *(ads) occur without transition states, we might speculate
fast adsorption rates on *(ads). If we assume the sticking coefficients to be 1.0 for all the Si species on *(ads) and use Θ equal to 1.0 together with the same molar fractions as used in section 1.1, we will obtain the same growth rates as shown in section 1.1 which are too high in comparison to the experimental values. As we have discussed previously, the exaggeration in the growth rate is likely due to the following facts. 1) Θ has been assumed equal to its maximum value (Θ = 1.0) and 2) we have not taken desorption processes into account.

Table 5 The energies at 0 K and standard Gibbs free energies at 1600 °C of the adsorption processes and sticking coefficients on H(ads) and *(ads) on the C face of 4H–SiC. The (free) energies are presented in the unit of kJ/mol and calculated with respect to the energy of the reactant state at asymptote condition.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>ΔᵣE° (0 K)</th>
<th>ΔₜₛE° (0 K)</th>
<th>ΔᵣG° (1600 °C)</th>
<th>ΔₜₛG° (1600 °C)</th>
<th>S (1600 °C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R29: SiH(g) + H(ads) → SiH₂(ads)</td>
<td>-194</td>
<td>47</td>
<td>63</td>
<td>292</td>
<td>3 × 10⁻³</td>
</tr>
<tr>
<td>R30: SiH₂(g) + H(ads) → SiH₃(ads)</td>
<td>-238</td>
<td>61</td>
<td>56</td>
<td>350</td>
<td>6 × 10⁻⁵</td>
</tr>
<tr>
<td>R31: SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>-149</td>
<td>77</td>
<td>133</td>
<td>336</td>
<td>2 × 10⁻⁴</td>
</tr>
<tr>
<td>R32: SiHCl(g) + H(ads) → SiH₂Cl(ads)</td>
<td>-207</td>
<td>116</td>
<td>123</td>
<td>422</td>
<td>8 × 10⁻⁷</td>
</tr>
<tr>
<td>R33: SiCl₂(g) + H(ads) → SiHCl₂(ads)</td>
<td>-153</td>
<td>192</td>
<td>186</td>
<td>506</td>
<td>4 × 10⁻⁹</td>
</tr>
<tr>
<td>R34: SiH(g) + *(ads) → SiH(ads)</td>
<td>-341</td>
<td>-</td>
<td>-51</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>R35: SiH₂(g) + *(ads) → SiH₂(ads)</td>
<td>-301</td>
<td>-</td>
<td>-1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>R36: SiCl(g) + *(ads) → SiCl(ads)</td>
<td>-338</td>
<td>-</td>
<td>-25</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>R37: SiHCl(g) + *(ads) → SiHCl(ads)</td>
<td>-267</td>
<td>-</td>
<td>66</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>R38: SiCl₂(g) + *(ads) → SiCl₂(ads)</td>
<td>-212</td>
<td>-</td>
<td>129</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

a) Energies and free energies of reaction, b) energies and free energies of activation, c) sticking coefficients.
Table 6 The adsorption and desorption rate constants at 1600 °C of SiH, SiH₂, SiCl, SiHCl and SiCl₂ on H(ads) on the C face of 4H–SiC.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Adsorption rate constant a)</th>
<th>Desorption rate constant b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R29</td>
<td>SiH(g) + H(ads) → SiH₂(ads)</td>
<td>2</td>
</tr>
<tr>
<td>R30</td>
<td>SiH₂(g) + H(ads) → SiH₃(ads)</td>
<td>5 × 10⁻²</td>
</tr>
<tr>
<td>R31</td>
<td>SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>1 × 10⁻¹</td>
</tr>
<tr>
<td>R32</td>
<td>SiHCl(g) + H(ads) → SiH₂Cl(ads)</td>
<td>4 × 10⁻⁴</td>
</tr>
<tr>
<td>R33</td>
<td>SiCl₂(g) + H(ads) → SiHCl₂(ads)</td>
<td>2 × 10⁻⁶</td>
</tr>
</tbody>
</table>

a) The adsorption rate constants, $R_{ads}/pγ_g\Theta_s$, are calculated using Eq. 5-8. Here, the adsorption rate ($R_{ads}$) is in molecule per site per second. The total pressure ($p$) is in pascal. The gaseous molar fraction ($γ_g$) and the surface fraction ($\Theta_s$) are unitless. The surface area per site of H(ads) is assumed equal to $8.178 \times 10^{-20}$ m² which is the area per one lattice site on the C-face of 4H–SiC.

b) The desorption rate constants, $R_{de}/\Theta_s$, are calculated using Eq. 9-10. Here, the desorption rate ($R_{de}$) is in molecule per site per second. The surface fraction ($\Theta_s$) is unitless.
Figure 9. Top view and side view of a) the transition state and b) the product of SiH adsorption on H(ads) on the C-face of 4H-SiC.

3 Adsorptions of SiHₓFᵧ, SiHₓBrₓ and Si atoms. The Gibbs free energies (Δ𝑅𝐺°) of adsorptions of SiHₓFᵧ, SiHₓBrₓ and Si atoms on both the Si face and the C face of 4H-SiC are shown in Table 7 and 8. Similar to the previous sections, adsorptions are more favorable on a surface site with the presence of a dangling bond, i.e. CH₂(ads) and *(ads).

Adsorptions of Si atoms are shown to be the most thermodynamically favorable among all the Si species in the study. On the Si face, the Gibbs free energies (Δ𝑅𝐺°) of Si atom adsorptions on CH₃(ads) and CH₂(ads) are 24 and -48 kJ/mol at 1600 °C, which are the lowest Δ𝑅𝐺° among the set. Similarly, on the C face, Δ𝑅𝐺° of Si atom adsorptions on H(ads) and *(ads) are also smallest among the set, with Δ𝑅𝐺° of -7 and -109 kJ/mol at 1600 °C. Due to the change in the spin states, these reactions are spin-forbidden and the calculation of the reaction rates is beyond the scope of this study.

For the halide systems, the Gibbs free energies (Δ𝑅𝐺°) from smallest to largest are observed in the adsorptions of SiX, SiHX and SiX₂, for X being the halides. This is similar to what we previously
observed in the adsorptions of the Cl chemistry. As a result, we propose that SiX (for X being F, Cl and Br) are the major growth contributors to SiC among the SiHxXy species.

**Table 7** The energies (0 K) and standard Gibbs free energies (1600 °C) of the adsorption processes of Si atoms, SiF, SiHF, SiF2, SiBr, SiHBr and SiBr2 on CH3(ads) and CH2(ads) pre-deposited on the Si face of 4H–SiC. The (free) energies are presented in the unit of kJ/mol, calculated with respect to the energy of the reactant state at asymptote condition.

<table>
<thead>
<tr>
<th>R</th>
<th>Reaction</th>
<th>( \Delta_R E^o ) (^{a)}) (0 K)</th>
<th>( \Delta_R G^o ) (^{a)}) (1600 °C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R40</td>
<td>(^3)Si(g) + CH3(ads) → SiH-CH2(ads)</td>
<td>-217</td>
<td>24</td>
</tr>
<tr>
<td>R41</td>
<td>SiF(g) + CH3(ads) → SiHF-CH2(ads)</td>
<td>-127</td>
<td>139</td>
</tr>
<tr>
<td>R42</td>
<td>SiHF(g) + CH3(ads) → SiH2F-CH2(ads)</td>
<td>-192</td>
<td>120</td>
</tr>
<tr>
<td>R43</td>
<td>SiF2(g) + CH3(ads) → SiHF2-CH2(ads)</td>
<td>-138</td>
<td>167</td>
</tr>
<tr>
<td>R44</td>
<td>SiBr(g) + CH3(ads) → SiHBr-CH2(ads)</td>
<td>-120</td>
<td>135</td>
</tr>
<tr>
<td>R45</td>
<td>SiHBr(g) + CH3(ads) → SiH2Br-CH2(ads)</td>
<td>-180</td>
<td>133</td>
</tr>
<tr>
<td>R46</td>
<td>SiBr2(g) + CH3(ads) → SiHBr2-CH2(ads)</td>
<td>-130</td>
<td>184</td>
</tr>
<tr>
<td>R47</td>
<td>(^3)Si(g) + CH2(ads) → Si-CH2(ads)</td>
<td>-320</td>
<td>-48</td>
</tr>
<tr>
<td>R48</td>
<td>SiF(g) + CH2(ads) → SiF-CH2(ads)</td>
<td>-316</td>
<td>19</td>
</tr>
<tr>
<td>R49</td>
<td>SiHF(g) + CH2(ads) → SiHF-CH2(ads)</td>
<td>-225</td>
<td>110</td>
</tr>
<tr>
<td>R50</td>
<td>SiF2(g) + CH2(ads) → SiF2-CH2(ads)</td>
<td>-163</td>
<td>162</td>
</tr>
<tr>
<td>R51</td>
<td>SiBr(g) + CH2(ads) → SiBr-CH2(ads)</td>
<td>-304</td>
<td>35</td>
</tr>
<tr>
<td>R52</td>
<td>SiHBr(g) + CH2(ads) → SiHBr-CH2(ads)</td>
<td>-224</td>
<td>101</td>
</tr>
<tr>
<td>R53</td>
<td>SiBr2(g) + CH2(ads) → SiBr2-CH2(ads)</td>
<td>-189</td>
<td>139</td>
</tr>
</tbody>
</table>

\(^{a)}\) Energies and free energies of reaction.
Table 8 The energies (0 K) and standard Gibbs free energies (1600 °C) of the adsorption processes of Si atoms, SiF, SiHF, SiF₂, SiBr, SiHBr and SiBr₂ on H(ads) and *(ads) on the C face of 4H−SiC. The (free) energies are presented in the unit of kJ/mol, calculated with respect to the energy of the reactant state at asymptote condition.

<table>
<thead>
<tr>
<th>R</th>
<th>Reaction</th>
<th>Δᵣ𝐸° folly)</th>
<th>Δᵣ𝐺° folly)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(0 K)</td>
<td>(1600 °C)</td>
</tr>
<tr>
<td>R54</td>
<td>³Si(g) + H(ads) → SiH(ads)</td>
<td>-222</td>
<td>-7</td>
</tr>
<tr>
<td>R55</td>
<td>SiF(g) + H(ads) → SiHF(ads)</td>
<td>-161</td>
<td>107</td>
</tr>
<tr>
<td>R56</td>
<td>SiHF(g) + H(ads) → SiH₂F(ads)</td>
<td>-225</td>
<td>100</td>
</tr>
<tr>
<td>R57</td>
<td>SiF₂(g) + H(ads) → SiHF₂(ads)</td>
<td>-175</td>
<td>156</td>
</tr>
<tr>
<td>R58</td>
<td>SiBr(g) + H(ads) → SiHBr(ads)</td>
<td>-148</td>
<td>135</td>
</tr>
<tr>
<td>R59</td>
<td>SiHBr(g) + H(ads) → SiH₂Br(ads)</td>
<td>-204</td>
<td>134</td>
</tr>
<tr>
<td>R60</td>
<td>SiBr₂(g) + H(ads) → SiHBr₂(ads)</td>
<td>-142</td>
<td>194</td>
</tr>
<tr>
<td>R61</td>
<td>³Si(g) + *(ads) → Si(ads)</td>
<td>-351</td>
<td>-109</td>
</tr>
<tr>
<td>R62</td>
<td>SiF(g) + *(ads) → SiF(ads)</td>
<td>-355</td>
<td>-44</td>
</tr>
<tr>
<td>R63</td>
<td>SiHF(g) + *(ads) → SiHF(ads)</td>
<td>-275</td>
<td>44</td>
</tr>
<tr>
<td>R64</td>
<td>SiF₂(g) + *(ads) → SiF₂(ads)</td>
<td>-215</td>
<td>108</td>
</tr>
<tr>
<td>R65</td>
<td>SiBr(g) + *(ads) → SiBr(ads)</td>
<td>-335</td>
<td>-10</td>
</tr>
<tr>
<td>R66</td>
<td>SiHBr(g) + *(ads) → SiHBr(ads)</td>
<td>-268</td>
<td>67</td>
</tr>
<tr>
<td>R67</td>
<td>SiBr₂(g) + *(ads) → SiBr₂(ads)</td>
<td>-211</td>
<td>133</td>
</tr>
</tbody>
</table>

Summary and Conclusion

The density functional theory (B3LYP and M06-2X) and transition state theory are used to study adsorption processes of active Si species on the Si face and the C face of 4H-SiC. On the Si face,
we show that adsorptions of SiCl, SiCl₂, SiHCl, SiH and SiH₂ occurs more likely on a methylene site, CH₂(ads). The processes are shown to occur without the presence of transition states and thus relatively large sticking probabilities should be expected. The $\Delta R G^\circ$ from smallest to largest are SiH $>$ SiCl $>$ SiH₂ $>$ SiHCl $>$ SiCl₂. Adsorptions on a methyl site, CH₃(ads), and on an ethylene site, C₂H₄(ads), both occur with relatively large activation barriers at the CVD process condition resulting in small sticking probabilities of all Si species considered. The adsorptions on CH₂(ads), CH₃(ads) as well as C₂H₄(ads) are all shown to be thermodynamically less favorable than their reverse, i.e. desorptions. The adsorbed products are shown to be stabilized by reacting with adjacent methyl sites and forming a larger cluster. These subsequent processes happen with rates that are fast enough to compete with desorption processes. On the C face, the adsorptions likely occur on a surface site terminated by a dangling bond, *(ads), which are shown to occur without the presence of transition states and produce stable products. The $\Delta R G^\circ$ from smallest to largest are SiH $>$ SiCl $>$ SiH₂ $>$ SiHCl $>$ SiCl₂. Lastly, we present the Gibbs free energies of adsorptions of Si atoms, SiX, SiX₂, SiHX, for X being F and Br. Again, it is observed that adsorptions on the Si face occurs most likely on a methylene site, CH₂(ads), while adsorptions on the C face occur on a surface site terminated by a dangling bond, *(ads). Adsorptions of Si atoms are shown to be the most thermodynamically favorable among all the species in the study. Among the halide-containing species, the Gibbs free energies ($\Delta R G^\circ$) from smallest to largest are observed in the adsorptions of SiX, SiHX and SiX₂, for X being the halides. From the results obtained in this study we conclude that the major Si contributors in the SiC-CVD process are Si atoms, SiX (for X being the halide) and SiH. This is unlike Si-CVD processes in which SiH₂ was predicted to be the most important species contributing to Si deposition²⁶,²⁷. The results also imply that SiX₂ is not a major contributor to SiC growth, in contrast to previous assumptions.
Supporting Information

Gibbs free energies, sticking coefficients, rate constants at the temperature range of 298 – 2500 K and molecular coordinates. This material is available free of charge via the internet at http://pubs.acs.org.

Corresponding Authors

*Emails: pitsu@ifm.liu.se and lars@ifm.liu.se.

Acknowledgment

The authors acknowledge financial support from the Swedish Foundation for Strategic Research, from the Swedish Government Strategic Research Area in Materials Science on Functional Materials at Linköping University (Faculty Grant SFO Mat LiU No 2009 00971), and from the Swedish Research Council (VR Grant No. 2016-05137_4). Supercomputer resources were provided by the Swedish National Infrastructure for Computing (SNIC) and the National Supercomputer Centre (NSC), Linköping University.

References


Supporting Information for

Growth Mechanism of SiC CVD – Adsorption and Surface Reactions of Active Si Species

Pitsiri Sukkaew*, Emil Kalered, Erik Janzén, Olof Kordina, Örjan Danielsson and Lars Ojamäe*

Department of Physics, Chemistry and Biology, Linköping University, SE-581 83 Linköping, Sweden

*Emails: pitsu@ifm.liu.se and lars@ifm.liu.se.
Table S1 Gibbs free energies of reaction ($\Delta G^\circ_R$) in kJ/mol at the temperature range of 298 – 2500 K.

\[
\Delta G^\circ_R = a_1 T^4 + a_2 T^3 + a_3 T^2 + a_4 T + a_5
\]
for temperature (T) = 298 – 2500 K.

<table>
<thead>
<tr>
<th></th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>SiH(g) + CH₃(ads) → SiH₂-CH₂(ads)</td>
<td>-2.87E-13</td>
<td>2.95E-09</td>
<td>-1.42E-05</td>
<td>1.54E-01</td>
</tr>
<tr>
<td>R2</td>
<td>SiH₂(g) + CH₃(ads) → SiH₁-CH₂(ads)</td>
<td>-1.37E-13</td>
<td>2.03E-09</td>
<td>-1.31E-05</td>
<td>1.79E-01</td>
</tr>
<tr>
<td>R3</td>
<td>SiCl(g) + CH₃(ads) → SiHCl-CH₂(ads)</td>
<td>-4.63E-13</td>
<td>4.20E-09</td>
<td>-1.76E-05</td>
<td>1.67E-01</td>
</tr>
<tr>
<td>R4</td>
<td>SiHCl(g) + CH₃(ads) → SiH₂Cl-CH₂(ads)</td>
<td>-3.29E-13</td>
<td>3.35E-09</td>
<td>-1.65E-05</td>
<td>1.93E-01</td>
</tr>
<tr>
<td>R5</td>
<td>SiCl₂(g) + CH₃(ads) → SiHCl₂-CH₂(ads)</td>
<td>-5.67E-13</td>
<td>5.03E-09</td>
<td>-2.10E-05</td>
<td>1.93E-01</td>
</tr>
<tr>
<td>R6</td>
<td>SiH(g) + CH₂(ads) → SiH₂-CH₂(ads)</td>
<td>5.36E-13</td>
<td>-2.93E-09</td>
<td>1.84E-06</td>
<td>1.86E-01</td>
</tr>
<tr>
<td>R7</td>
<td>SiH₂(g) + CH₂(ads) → SiH₂-CH₂(ads)</td>
<td>3.17E-13</td>
<td>-1.36E-09</td>
<td>-3.24E-06</td>
<td>1.79E-01</td>
</tr>
<tr>
<td>R8</td>
<td>SiCl(g) + CH₂(ads) → SiCl₂-CH₂(ads)</td>
<td>2.12E-13</td>
<td>-7.33E-10</td>
<td>-3.66E-06</td>
<td>1.93E-01</td>
</tr>
<tr>
<td>R9</td>
<td>SiHCl(g) + CH₂(ads) → SiHCl₂-CH₂(ads)</td>
<td>2.58E-13</td>
<td>-9.36E-10</td>
<td>-4.42E-06</td>
<td>1.94E-01</td>
</tr>
<tr>
<td>R10</td>
<td>SiCl₂(g) + CH₂(ads) → SiCl₂-CH₂(ads)</td>
<td>-5.17E-14</td>
<td>1.23E-09</td>
<td>-1.01E-05</td>
<td>1.82E-01</td>
</tr>
<tr>
<td>R11</td>
<td>SiH(g) + C₂H₄(ads) → SiH-((CH₂)₂)ads</td>
<td>-3.25E-13</td>
<td>2.92E-09</td>
<td>-1.28E-05</td>
<td>1.60E-01</td>
</tr>
<tr>
<td>R12</td>
<td>SiH₂(g) + C₂H₄(ads) → SiH₂-(CH₂)₂ads</td>
<td>-2.19E-13</td>
<td>2.35E-09</td>
<td>-1.28E-05</td>
<td>1.80E-01</td>
</tr>
<tr>
<td>R13</td>
<td>SiCl(g) + C₂H₄(ads) → SiCl-(CH₂)₂ads</td>
<td>-6.34E-13</td>
<td>5.07E-09</td>
<td>-1.83E-05</td>
<td>1.72E-01</td>
</tr>
<tr>
<td>R14</td>
<td>SiHCl(g) + C₂H₄(ads) → SiHCl-(CH₂)₂ads</td>
<td>-5.08E-13</td>
<td>4.35E-09</td>
<td>-1.79E-05</td>
<td>1.94E-01</td>
</tr>
<tr>
<td>R15</td>
<td>SiCl₂(g) + C₂H₄(ads) → SiCl₂-(CH₂)₂ads</td>
<td>-7.43E-13</td>
<td>5.97E-09</td>
<td>-2.21E-05</td>
<td>1.98E-01</td>
</tr>
<tr>
<td>R17</td>
<td>C₂H₄(ads) + H(g) → CH₃(ads) + CH₃(ads)</td>
<td>-1.55E-13</td>
<td>7.55E-10</td>
<td>-1.21E-06</td>
<td>7.50E-02</td>
</tr>
<tr>
<td>R18</td>
<td>SiH-CH₂(ads) + CH₃(ads) → SiH₂-(CH₂)₂(ads)</td>
<td>3.94E-13</td>
<td>-2.44E-09</td>
<td>5.02E-06</td>
<td>3.13E-02</td>
</tr>
<tr>
<td></td>
<td>Reaction</td>
<td>E0</td>
<td>E1</td>
<td>E2</td>
<td>E3</td>
</tr>
<tr>
<td>---</td>
<td>--------------------------------------------------------------------------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>R19</td>
<td>SiH$_3$-CH$_2$(ads) + CH$_3$(ads) → SiH$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>-3.20E-13</td>
<td>2.56E-09</td>
<td>-7.37E-06</td>
<td>-6.61E-02</td>
</tr>
<tr>
<td>R20</td>
<td>SiCl-CH$_3$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads)</td>
<td>3.17E-13</td>
<td>-1.88E-09</td>
<td>3.42E-06</td>
<td>2.25E-02</td>
</tr>
<tr>
<td>R21</td>
<td>SiHCl-CH$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads) + H(g)</td>
<td>-4.83E-13</td>
<td>3.65E-09</td>
<td>-1.01E-05</td>
<td>-6.65E-02</td>
</tr>
<tr>
<td>R22</td>
<td>SiCl$_2$-CH$_2$(ads) + CH$_3$(ads) → SiCl$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>-5.09E-13</td>
<td>3.82E-09</td>
<td>-1.05E-05</td>
<td>-6.73E-02</td>
</tr>
<tr>
<td>R23</td>
<td>SiH$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads) + H$_2$(g)</td>
<td>-8.77E-13</td>
<td>5.67E-09</td>
<td>-1.02E-05</td>
<td>-9.83E-02</td>
</tr>
<tr>
<td>R24</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiH-(CH$_2$)$_2$(ads) + HCl(g)</td>
<td>1.69E-13</td>
<td>-1.51E-09</td>
<td>7.59E-06</td>
<td>-1.26E-01</td>
</tr>
<tr>
<td>R25</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiH-(CH$_2$)$_2$(ads) + HCl(g)</td>
<td>-8.65E-13</td>
<td>5.58E-09</td>
<td>-9.89E-06</td>
<td>-8.92E-02</td>
</tr>
<tr>
<td>R26</td>
<td>SiCl$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiCl$_2$-(CH$_2$)$_2$(ads) + H$_2$(g)</td>
<td>3.23E-13</td>
<td>-2.60E-09</td>
<td>1.05E-05</td>
<td>-1.22E-01</td>
</tr>
<tr>
<td>R27</td>
<td>SiH-(CH$_2$)$_2$(ads) + H(g) → Si*(CH$_2$)$_2$(ads) + H$_2$(g)</td>
<td>-3.24E-13</td>
<td>1.42E-09</td>
<td>1.89E-06</td>
<td>-1.56E-02</td>
</tr>
<tr>
<td>R28</td>
<td>SiCl-(CH$_2$)$_2$(ads) + H(g) → Si*(CH$_2$)$_2$(ads) + HCl(g)</td>
<td>7.10E-13</td>
<td>-5.66E-09</td>
<td>1.94E-05</td>
<td>-5.25E-02</td>
</tr>
<tr>
<td>R29</td>
<td>SiH(g) + H(ads) → SiH$_2$(ads)</td>
<td>-3.13E-13</td>
<td>2.98E-09</td>
<td>-1.36E-05</td>
<td>1.56E-01</td>
</tr>
<tr>
<td>R30</td>
<td>SiH$_2$(g) + H(ads) → SiH$_3$(ads)</td>
<td>-1.34E-13</td>
<td>1.91E-09</td>
<td>-1.23E-05</td>
<td>1.77E-01</td>
</tr>
<tr>
<td>R31</td>
<td>SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>-5.63E-13</td>
<td>4.71E-09</td>
<td>-1.81E-05</td>
<td>1.73E-01</td>
</tr>
<tr>
<td>R32</td>
<td>SiHCl(g) + H(ads) → SiH$_2$Cl(ads)</td>
<td>-3.38E-13</td>
<td>3.29E-09</td>
<td>-1.57E-05</td>
<td>1.98E-01</td>
</tr>
<tr>
<td>R33</td>
<td>SiCl$_2$(g) + H(ads) → SiHCl$_2$(ads)</td>
<td>-5.34E-13</td>
<td>4.68E-09</td>
<td>-1.94E-05</td>
<td>2.06E-01</td>
</tr>
<tr>
<td>R34</td>
<td>SiH(g) + *(ads) → SiH(ads)</td>
<td>-7.35E-14</td>
<td>1.18E-09</td>
<td>-8.24E-06</td>
<td>1.69E-01</td>
</tr>
<tr>
<td>R35</td>
<td>SiH$_2$(g) + *(ads) → SiH$_2$(ads)</td>
<td>-1.57E-13</td>
<td>1.90E-09</td>
<td>-1.15E-05</td>
<td>1.79E-01</td>
</tr>
<tr>
<td>R36</td>
<td>SiCl(g) + *(ads) → SiCl(ads)</td>
<td>-3.19E-13</td>
<td>2.83E-09</td>
<td>-1.23E-05</td>
<td>1.83E-01</td>
</tr>
<tr>
<td>Reaction</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>----------------</td>
<td>----------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R37</td>
<td>SiHCl(g) + *(ads) → SiHCl(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R38</td>
<td>SiCl2(g) + *(ads) → SiCl2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R40</td>
<td>3Si(g) + CH2(ads) → SiH-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R41</td>
<td>SiF(g) + CH2(ads) → SiHF-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R42</td>
<td>SiHF(g) + CH2(ads) → SiH2F-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R43</td>
<td>SiF3(g) + CH2(ads) → SiHF2-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R44</td>
<td>SiBr(g) + CH2(ads) → SiHBr-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R45</td>
<td>SiHBr(g) + CH2(ads) → SiH2Br-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R46</td>
<td>SiBr2(g) + CH2(ads) → SiHBr2-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R47</td>
<td>3Si(g) + CH2(ads) → Si-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R48</td>
<td>SiF(g) + CH2(ads) → SiF-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R49</td>
<td>SiHF(g) + CH2(ads) → SiHF-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R50</td>
<td>SiF2(g) + CH2(ads) → SiF2-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R51</td>
<td>SiBr(g) + CH2(ads) → SiBr-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R52</td>
<td>SiHBr(g) + CH2(ads) → SiHBr-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R53</td>
<td>SiBr2(g) + CH2(ads) → SiBr2-CH2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R54</td>
<td>3Si(g) + H(ads) → SiH(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R55</td>
<td>SiF(g) + H(ads) → SiHF(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R56</td>
<td>SiHF(g) + H(ads) → SiH2F(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R57</td>
<td>SiF2(g) + H(ads) → SiHF2(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R58</td>
<td>SiBr(g) + H(ads) → SiHBr(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R59</td>
<td>SiHBr(g) + H(ads) → SiH2Br(ads)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| Energy (kJ/mol) | | | | | |
|----------------|----------------|
| -2.87E-13 | 2.79E-09 | -1.37E-05 | 1.98E-01 | -2.70E+02 |
\[ \Delta G^\dagger = a_1T^4 + a_2T^3 + a_3T^2 + a_4T + a_5 \] for temperature (T) = 298 – 2500 K.

Table S2 Gibbs free energies of activation in kJ/mol at the temperature range of 298 – 2500 K.

<table>
<thead>
<tr>
<th>R</th>
<th>Reaction</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( a_3 )</th>
<th>( a_4 )</th>
<th>( a_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>R60</td>
<td>SiBr(_2)(g) + H(ads) → SiHBr(_2)(ads)</td>
<td>-6.27E-13</td>
<td>5.30E-09</td>
<td>-2.10E-05</td>
<td>2.05E-01</td>
<td>-1.43E+02</td>
</tr>
<tr>
<td>R61</td>
<td>(^3)Si(ads) + *(ads) → Si(ads)</td>
<td>-7.90E-14</td>
<td>7.76E-10</td>
<td>-3.78E-06</td>
<td>1.35E-01</td>
<td>-3.54E+02</td>
</tr>
<tr>
<td>R62</td>
<td>SiF(ads) + *(ads) → SiF(ads)</td>
<td>-2.90E-13</td>
<td>2.63E-09</td>
<td>-1.18E-05</td>
<td>1.82E-01</td>
<td>-3.58E+02</td>
</tr>
<tr>
<td>R63</td>
<td>SiHF(ads) + *(ads) → SiHF(ads)</td>
<td>-3.09E-13</td>
<td>2.95E-09</td>
<td>-1.42E-05</td>
<td>1.90E-01</td>
<td>-2.78E+02</td>
</tr>
<tr>
<td>R64</td>
<td>SiF(_2)(ads) + *(ads) → SiF(_2)(ads)</td>
<td>-4.33E-13</td>
<td>3.79E-09</td>
<td>-1.64E-05</td>
<td>1.94E-01</td>
<td>-2.17E+02</td>
</tr>
<tr>
<td>R65</td>
<td>SiBr(ads) + *(ads) → SiBr(ads)</td>
<td>-2.20E-13</td>
<td>2.13E-09</td>
<td>-1.05E-05</td>
<td>1.88E-01</td>
<td>-3.37E+02</td>
</tr>
<tr>
<td>R66</td>
<td>SiHBr(ads) + *(ads) → SiHBr(ads)</td>
<td>-3.02E-13</td>
<td>2.89E-09</td>
<td>-1.40E-05</td>
<td>1.98E-01</td>
<td>-2.71E+02</td>
</tr>
<tr>
<td>R67</td>
<td>SiBr(_2)(ads) + *(ads) → SiBr(_2)(ads)</td>
<td>-4.78E-13</td>
<td>4.10E-09</td>
<td>-1.70E-05</td>
<td>2.05E-01</td>
<td>-2.12E+02</td>
</tr>
<tr>
<td>R14</td>
<td>SiHCl(g) + C_2H_4(ads) → SiHCl-(CH_2)_2(ads)</td>
<td>-9.87E-13</td>
<td>7.22E-09</td>
<td>-2.18E-05</td>
<td>1.73E-01</td>
<td>2.34E+02</td>
</tr>
<tr>
<td>R15</td>
<td>SiCl_2(g) + C_2H_4(ads) → SiCl_2-(CH_2)_2(ads)</td>
<td>-1.20E-12</td>
<td>8.65E-09</td>
<td>-2.53E-05</td>
<td>1.71E-01</td>
<td>2.78E+02</td>
</tr>
<tr>
<td>R18</td>
<td>SiH-CH_2(ads) + CH_3(ads) → SiH-(CH_2)_2(ads)</td>
<td>2.85E-13</td>
<td>-2.08E-09</td>
<td>7.37E-06</td>
<td>2.31E-02</td>
<td>9.17E+01</td>
</tr>
<tr>
<td>R19</td>
<td>SiH_2-CH_2(ads) + CH_3(ads) → SiH_2-(CH_2)_2(ads) + H(g)</td>
<td>1.72E-13</td>
<td>-1.03E-09</td>
<td>3.51E-06</td>
<td>3.51E-02</td>
<td>1.73E+02</td>
</tr>
<tr>
<td>R20</td>
<td>SiCl-CH_2(ads) + CH_3(ads) → SiHCl-(CH_2)_2(ads)</td>
<td>1.75E-13</td>
<td>-1.30E-09</td>
<td>5.24E-06</td>
<td>1.27E-02</td>
<td>1.41E+02</td>
</tr>
<tr>
<td>R21</td>
<td>SiHCl-CH_2(ads) + CH_3(ads) → SiHCl-(CH_2)_2(ads) + H(g)</td>
<td>1.05E-13</td>
<td>-5.95E-10</td>
<td>2.48E-06</td>
<td>3.52E-02</td>
<td>1.63E+02</td>
</tr>
<tr>
<td>R22</td>
<td>SiCl_2-CH_2(ads) + CH_3(ads) → SiCl_2-(CH_2)_2(ads) + H(g)</td>
<td>9.10E-15</td>
<td>2.02E-10</td>
<td>-2.47E-07</td>
<td>2.16E-02</td>
<td>1.87E+02</td>
</tr>
<tr>
<td>R23</td>
<td>SiH_2-(CH_2)_2(ads) + CH_3(ads) → SiH-(CH_2)_3(ads) + H_2(g)</td>
<td>1.06E-13</td>
<td>-4.55E-10</td>
<td>1.42E-06</td>
<td>8.37E-03</td>
<td>2.90E+02</td>
</tr>
<tr>
<td>R24</td>
<td>SiHCl-(CH_2)_2(ads) + CH_3(ads) → SiH-(CH_2)_3(ads) + HCl(g)</td>
<td>2.71E-13</td>
<td>-2.01E-09</td>
<td>7.14E-06</td>
<td>1.33E-02</td>
<td>2.29E+02</td>
</tr>
<tr>
<td>R25</td>
<td>SiHCl-(CH_2)_3(ads) + CH_3(ads) → SiCl-(CH_2)_3(ads) + HCl(g)</td>
<td>1.16E-13</td>
<td>-6.45E-10</td>
<td>2.42E-06</td>
<td>9.80E-03</td>
<td>2.65E+02</td>
</tr>
<tr>
<td>R26</td>
<td>SiCl-(CH_2)_2(ads) + CH_3(ads) → SiCl-(CH_2)_3(ads) + HCl(g)</td>
<td>5.25E-13</td>
<td>-3.65E-09</td>
<td>1.09E-05</td>
<td>1.45E-02</td>
<td>2.40E+02</td>
</tr>
<tr>
<td>R27</td>
<td>SiH-(CH_2)_3(ads) + H(g) → Si*-(-(CH_2)_3(ads) + H_2(g)</td>
<td>1.95E-13</td>
<td>-1.46E-09</td>
<td>5.04E-06</td>
<td>8.58E-02</td>
<td>9.45E+00</td>
</tr>
<tr>
<td>R28</td>
<td>SiCl-(CH_2)_3(ads) + H(g) → Si*--(CH_2)_3(ads) + HCl(g)</td>
<td>3.24E-13</td>
<td>-2.40E-09</td>
<td>7.67E-06</td>
<td>8.36E-02</td>
<td>8.60E+01</td>
</tr>
<tr>
<td>R29</td>
<td>SiH(g) + H(ads) → SiH_2(ads)</td>
<td>-3.92E-13</td>
<td>3.16E-09</td>
<td>-1.09E-05</td>
<td>1.44E-01</td>
<td>4.48E+01</td>
</tr>
<tr>
<td>R30</td>
<td>SiH_2(g) + H(ads) → SiH_3(ads)</td>
<td>-3.15E-13</td>
<td>2.75E-09</td>
<td>-1.11E-05</td>
<td>1.70E-01</td>
<td>5.73E+01</td>
</tr>
<tr>
<td>R31</td>
<td>SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>-6.32E-13</td>
<td>4.81E-09</td>
<td>-1.51E-05</td>
<td>1.54E-01</td>
<td>7.82E+01</td>
</tr>
<tr>
<td>R32</td>
<td>SiHCl(g) + H(ads) → SiH_2Cl(ads)</td>
<td>-6.07E-13</td>
<td>4.72E-09</td>
<td>-1.60E-05</td>
<td>1.82E-01</td>
<td>1.15E+02</td>
</tr>
</tbody>
</table>
Table S3 Sticking coefficients, $S = AT^n \exp(-E/RT)$, at the temperature range of 298 – 2500 K. The energy (E) is in the unit of kJ/mol.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$S$ (1600 °C)</th>
<th>$298 – 2500 K$</th>
<th>ln (A)</th>
<th>n</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>SiH(g) + CH₃(ads) → SiH₂-CH₂(ads)</td>
<td>3.02E-04</td>
<td>-22.215</td>
<td>2.524</td>
<td>76.516</td>
</tr>
<tr>
<td>R2</td>
<td>SiH₂(g) + CH₃(ads) → SiH₃-CH₂(ads)</td>
<td>2.60E-05</td>
<td>-25.921</td>
<td>2.727</td>
<td>80.711</td>
</tr>
<tr>
<td>R3</td>
<td>SiCl(g) + CH₃(ads) → SiHCl-CH₂(ads)</td>
<td>4.33E-05</td>
<td>-23.879</td>
<td>2.716</td>
<td>103.288</td>
</tr>
<tr>
<td>R4</td>
<td>SiHCl(g) + CH₃(ads) → SiHCl₂-CH₂(ads)</td>
<td>7.03E-07</td>
<td>-28.371</td>
<td>2.889</td>
<td>117.891</td>
</tr>
<tr>
<td>R5</td>
<td>SiCl₂(g) + CH₃(ads) → SiClH₂-CH₂(ads)</td>
<td>8.15E-09</td>
<td>-29.411</td>
<td>3.018</td>
<td>186.254</td>
</tr>
<tr>
<td>R11</td>
<td>SiH(g) + C₂H₄(ads) → SiH-(CH₂)₂(ads)</td>
<td>9.48E-06</td>
<td>-20.860</td>
<td>2.397</td>
<td>136.556</td>
</tr>
<tr>
<td>R12</td>
<td>SiH₂(g) + C₂H₄(ads) → SiH₂-(CH₂)₂(ads)</td>
<td>5.31E-08</td>
<td>-24.845</td>
<td>2.795</td>
<td>202.007</td>
</tr>
<tr>
<td>R13</td>
<td>SiCl(g) + C₂H₄(ads) → SiCl-(CH₂)₂(ads)</td>
<td>6.61E-06</td>
<td>-21.531</td>
<td>2.533</td>
<td>147.736</td>
</tr>
<tr>
<td>R14</td>
<td>SiHCl(g) + C₂H₄(ads) → SiHCl-(CH₂)₂(ads)</td>
<td>1.68E-09</td>
<td>-27.043</td>
<td>2.883</td>
<td>231.808</td>
</tr>
<tr>
<td>R15</td>
<td>SiCl₂(g) + C₂H₄(ads) → SiCl₂-(CH₂)₂(ads)</td>
<td>1.98E-10</td>
<td>-27.388</td>
<td>3.019</td>
<td>275.674</td>
</tr>
<tr>
<td>R29</td>
<td>SiH(g) + H(ads) → SiH₂(ads)</td>
<td>2.62E-03</td>
<td>-20.912</td>
<td>2.355</td>
<td>43.270</td>
</tr>
<tr>
<td>R30</td>
<td>SiH₂(g) + H(ads) → SiH₃(ads)</td>
<td>6.35E-05</td>
<td>-25.508</td>
<td>2.572</td>
<td>55.036</td>
</tr>
<tr>
<td>R31</td>
<td>SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>1.88E-04</td>
<td>-22.666</td>
<td>2.523</td>
<td>76.678</td>
</tr>
<tr>
<td>R32</td>
<td>SiHCl(g) + H(ads) → SiH₂Cl(ads)</td>
<td>7.69E-07</td>
<td>-27.618</td>
<td>2.754</td>
<td>112.348</td>
</tr>
<tr>
<td>R33</td>
<td>SiCl₂(g) + H(ads) → SiHCl₂(ads)</td>
<td>3.67E-09</td>
<td>-28.940</td>
<td>2.881</td>
<td>189.888</td>
</tr>
</tbody>
</table>
Table S4 Rate constants in forward and reverse directions. A and E are in the units of molecules per site per second and kJ/mol.

<table>
<thead>
<tr>
<th></th>
<th>Forward rate constants</th>
<th>Reverse rate constants</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ln (A)</td>
<td>n</td>
</tr>
<tr>
<td>R18</td>
<td>SiH-CH$_2$(ads) + CH$_3$(ads) → SiH$_2$-(CH$_2$)$_2$(ads)</td>
<td>25.088</td>
</tr>
<tr>
<td>R19</td>
<td>SiH$_2$-CH$_2$(ads) + CH$_3$(ads) → SiH$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>21.913</td>
</tr>
<tr>
<td>R20</td>
<td>SiCl-CH$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads)</td>
<td>25.760</td>
</tr>
<tr>
<td>R21</td>
<td>SiHCl-CH$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_2$(ads) + H(g)</td>
<td>21.767</td>
</tr>
<tr>
<td>R22</td>
<td>SiCl$_2$-CH$_2$(ads) + CH$_3$(ads) → SiCl$_2$-(CH$_2$)$_2$(ads) + H(g)</td>
<td>22.261</td>
</tr>
<tr>
<td>R23</td>
<td>SiH$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiH-(CH$_2$)$_3$(ads) + H$_2$(g)</td>
<td>24.102</td>
</tr>
<tr>
<td>R24</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiHCl-(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>26.089</td>
</tr>
<tr>
<td>R25</td>
<td>SiHCl-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiCl-(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>24.630</td>
</tr>
<tr>
<td>R26</td>
<td>SiCl$_2$-(CH$_2$)$_2$(ads) + CH$_3$(ads) → SiCl-(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>25.932</td>
</tr>
<tr>
<td>R27</td>
<td>SiH-(CH$_2$)$_3$(ads) + H(g) → Si*(CH$_2$)$_3$(ads) + H$_2$(g)</td>
<td>6.449</td>
</tr>
<tr>
<td>R28</td>
<td>SiCl-(CH$_2$)$_3$(ads) + H(g) → Si*(CH$_2$)$_3$(ads) + HCl(g)</td>
<td>6.141</td>
</tr>
<tr>
<td>R29</td>
<td>SiH(g) + H(ads) → SiH$_2$(ads)</td>
<td>-10.563</td>
</tr>
<tr>
<td>R30</td>
<td>SiH$_3$(g) + H(ads) → SiH$_3$(ads)</td>
<td>-15.192</td>
</tr>
<tr>
<td>R31</td>
<td>SiCl(g) + H(ads) → SiHCl(ads)</td>
<td>-12.736</td>
</tr>
<tr>
<td>R32</td>
<td>SiHCl(g) + H(ads) → SiH$_3$Cl(ads)</td>
<td>-17.679</td>
</tr>
</tbody>
</table>
\[
\text{R33: } \text{SiCl}_2(g) + \text{H(ads)} \rightarrow \text{SiHCl}_2(\text{ads})
\]

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>-19.224</td>
<td>2.413</td>
<td>190.480</td>
<td>29.782</td>
<td>0.449</td>
<td>349.358</td>
</tr>
</tbody>
</table>

**Table S4 Molecular Coordinates in Z-matrix form**

CH$_3$(ads)

<p>| | | | | |
| | | | | |
|---|---|---|---|
| Si | 1 | B1 | |
| Si | 2 | B3 | 1 | A2 | 3 | D1 |
| Si | 2 | B4 | 1 | A3 | 3 | D2 |
| Si | 5 | B5 | 2 | A4 | 1 | D3 |
| Si | 3 | B6 | 1 | A5 | 6 | D4 |
| Si | 2 | B7 | 1 | A6 | 3 | D5 |
| Si | 2 | B8 | 1 | A7 | 3 | D6 |
| Si | 7 | B9 | 3 | A8 | 1 | D7 |
| Si | 9 | B10 | 2 | A9 | 1 | D8 |
| Si | 3 | B11 | 1 | A10 | 6 | D9 |
| C | 6 | B12 | 5 | A11 | 2 | D10 |
| C | 1 | B13 | 3 | A12 | 12 | D11 |
| C | 2 | B14 | 1 | A13 | 14 | D12 |
| C | 12 | B15 | 3 | A14 | 1 | D13 |
| C | 11 | B16 | 9 | A15 | 2 | D14 |
| C | 10 | B17 | 7 | A16 | 3 | D15 |
| C | 7 | B18 | 3 | A17 | 1 | D16 |
| C | 12 | B19 | 3 | A18 | 1 | D17 |
| C | 7 | B20 | 3 | A19 | 1 | D18 |
| C | 9 | B21 | 2 | A20 | 1 | D19 |
| H | 1 | B22 | 14 | A21 | 3 | D20 |
| H | 2 | B23 | 1 | A22 | 14 | D21 |
| H | 3 | B24 | 1 | A23 | 14 | D22 |
| H | 5 | B25 | 2 | A24 | 1 | D23 |
| H | 16 | B26 | 12 | A25 | 3 | D24 |
| H | 6 | B27 | 5 | A26 | 2 | D25 |
| H | 17 | B28 | 11 | A27 | 9 | D26 |
| H | 18 | B29 | 10 | A28 | 7 | D27 |
| H | 19 | B30 | 7 | A29 | 3 | D28 |
| H | 20 | B31 | 12 | A30 | 3 | D29 |
| H | 21 | B32 | 7 | A31 | 3 | D30 |
| H | 22 | B33 | 9 | A32 | 2 | D31 |
| C | 4 | B34 | 2 | A33 | 1 | D32 |
| C | 3 | B35 | 1 | A34 | 14 | D33 |
| Si | 20 | B36 | 12 | A35 | 3 | D34 |
| Si | 19 | B37 | 7 | A36 | 3 | D35 |
| C | 38 | B38 | 19 | A37 | 7 | D36 |
| Si | 36 | B39 | 3 | A38 | 1 | D37 |
| H | 39 | B40 | 38 | A39 | 19 | D38 |
| H | 39 | B41 | 38 | A40 | 19 | D39 |
| H | 40 | B42 | 36 | A41 | 3 | D40 |
| H | 40 | B43 | 36 | A42 | 3 | D41 |</p>
<table>
<thead>
<tr>
<th>Column</th>
<th>Row</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>43</td>
<td>7</td>
</tr>
<tr>
<td>B</td>
<td>44</td>
<td>19</td>
</tr>
<tr>
<td>C</td>
<td>50</td>
<td>14</td>
</tr>
<tr>
<td>Si</td>
<td>53</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>11</td>
<td>9</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>Si</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>22</td>
<td>9</td>
</tr>
<tr>
<td>H</td>
<td>17</td>
<td>11</td>
</tr>
<tr>
<td>H</td>
<td>21</td>
<td>7</td>
</tr>
<tr>
<td>H</td>
<td>18</td>
<td>10</td>
</tr>
<tr>
<td>H</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>H</td>
<td>1</td>
<td>14</td>
</tr>
<tr>
<td>Si</td>
<td>15</td>
<td>2</td>
</tr>
<tr>
<td>Si</td>
<td>35</td>
<td>4</td>
</tr>
<tr>
<td>C</td>
<td>37</td>
<td>20</td>
</tr>
<tr>
<td>C</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>15</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>35</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>35</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>15</td>
</tr>
<tr>
<td>C</td>
<td>64</td>
<td>35</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>37</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>37</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>8</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>8</td>
</tr>
<tr>
<td>Si</td>
<td>66</td>
<td>8</td>
</tr>
<tr>
<td>H</td>
<td>76</td>
<td>66</td>
</tr>
<tr>
<td>H</td>
<td>71</td>
<td>64</td>
</tr>
<tr>
<td>C</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>54</td>
<td>53</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>4</td>
</tr>
</tbody>
</table>

B1: 6.23695371  
B2: 3.12466288  
B3: 3.12492341  
B4: 3.123748  
B5: 3.11360127  
B6: 3.1524921  
B7: 3.1426496  
B8: 3.1508112  
B9: 3.14880025  
B10: 3.1549541  
B11: 3.13241433
<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>60.3985892</td>
</tr>
<tr>
<td>A2</td>
<td>60.2814074</td>
</tr>
<tr>
<td>A3</td>
<td>59.96071561</td>
</tr>
<tr>
<td>A4</td>
<td>120.1180162</td>
</tr>
<tr>
<td>A5</td>
<td>60.67280944</td>
</tr>
<tr>
<td>A6</td>
<td>90.82283311</td>
</tr>
<tr>
<td>A7</td>
<td>60.90594021</td>
</tr>
<tr>
<td>A8</td>
<td>90.22948376</td>
</tr>
<tr>
<td>A9</td>
<td>119.6288691</td>
</tr>
<tr>
<td>A10</td>
<td>90.30442162</td>
</tr>
<tr>
<td>A11</td>
<td>35.35788672</td>
</tr>
<tr>
<td>A12</td>
<td>35.0643815</td>
</tr>
<tr>
<td>A13</td>
<td>90.85770531</td>
</tr>
<tr>
<td>A14</td>
<td>121.4800106</td>
</tr>
<tr>
<td>A15</td>
<td>34.13570145</td>
</tr>
<tr>
<td>A16</td>
<td>146.5416694</td>
</tr>
<tr>
<td>A17</td>
<td>72.46894057</td>
</tr>
<tr>
<td>A18</td>
<td>121.4436956</td>
</tr>
<tr>
<td>A19</td>
<td>122.9357033</td>
</tr>
<tr>
<td>A20</td>
<td>75.28209501</td>
</tr>
<tr>
<td>A21</td>
<td>110.2257498</td>
</tr>
<tr>
<td>A22</td>
<td>90.30543783</td>
</tr>
<tr>
<td>A23</td>
<td>88.98135511</td>
</tr>
<tr>
<td>A24</td>
<td>90.33554663</td>
</tr>
<tr>
<td>A25</td>
<td>107.2155325</td>
</tr>
<tr>
<td>A26</td>
<td>88.99419571</td>
</tr>
<tr>
<td>A27</td>
<td>109.0221151</td>
</tr>
<tr>
<td>A28</td>
<td>108.2908169</td>
</tr>
<tr>
<td>A29</td>
<td>108.3601459</td>
</tr>
<tr>
<td>A30</td>
<td>107.4669778</td>
</tr>
<tr>
<td>A31</td>
<td>109.1951214</td>
</tr>
<tr>
<td>A32</td>
<td>108.4688791</td>
</tr>
<tr>
<td>A33</td>
<td>144.5375037</td>
</tr>
<tr>
<td>D5</td>
<td>-54.35051215</td>
</tr>
<tr>
<td>--------</td>
<td>--------------</td>
</tr>
<tr>
<td>D6</td>
<td>-109.1082648</td>
</tr>
<tr>
<td>D7</td>
<td>-54.37737111</td>
</tr>
<tr>
<td>D8</td>
<td>-69.94345952</td>
</tr>
<tr>
<td>D9</td>
<td>54.33324609</td>
</tr>
<tr>
<td>D10</td>
<td>142.1323596</td>
</tr>
<tr>
<td>D11</td>
<td>-87.799067</td>
</tr>
<tr>
<td>D12</td>
<td>1.74596961</td>
</tr>
<tr>
<td>D13</td>
<td>-13.6888881</td>
</tr>
<tr>
<td>D14</td>
<td>-109.5536475</td>
</tr>
<tr>
<td>D15</td>
<td>163.1627898</td>
</tr>
<tr>
<td>D16</td>
<td>-144.8243505</td>
</tr>
<tr>
<td>D17</td>
<td>-164.6299641</td>
</tr>
<tr>
<td>D18</td>
<td>-43.73605895</td>
</tr>
<tr>
<td>D19</td>
<td>142.5899682</td>
</tr>
<tr>
<td>D20</td>
<td>56.55185004</td>
</tr>
<tr>
<td>D21</td>
<td>112.1358392</td>
</tr>
<tr>
<td>D22</td>
<td>126.2021335</td>
</tr>
<tr>
<td>D23</td>
<td>-88.87939352</td>
</tr>
<tr>
<td>D24</td>
<td>143.9033332</td>
</tr>
<tr>
<td>D25</td>
<td>-89.77091013</td>
</tr>
<tr>
<td>D26</td>
<td>-119.6596729</td>
</tr>
<tr>
<td>D27</td>
<td>60.26658954</td>
</tr>
<tr>
<td>D28</td>
<td>178.887737</td>
</tr>
<tr>
<td>D29</td>
<td>-143.965859</td>
</tr>
<tr>
<td>D30</td>
<td>-138.8950368</td>
</tr>
<tr>
<td>D31</td>
<td>-176.6807499</td>
</tr>
<tr>
<td>D32</td>
<td>-144.1122691</td>
</tr>
<tr>
<td>D33</td>
<td>0.81035325</td>
</tr>
<tr>
<td>D34</td>
<td>-26.80460128</td>
</tr>
<tr>
<td>D35</td>
<td>-61.90128408</td>
</tr>
<tr>
<td>D36</td>
<td>-178.533856</td>
</tr>
<tr>
<td>D37</td>
<td>179.3429321</td>
</tr>
<tr>
<td>D38</td>
<td>174.7710776</td>
</tr>
<tr>
<td>D39</td>
<td>57.51704687</td>
</tr>
<tr>
<td>D40</td>
<td>-177.6577624</td>
</tr>
<tr>
<td>D41</td>
<td>-59.53794311</td>
</tr>
<tr>
<td>D42</td>
<td>-56.317336</td>
</tr>
<tr>
<td>D43</td>
<td>111.5786947</td>
</tr>
<tr>
<td>D44</td>
<td>61.39967194</td>
</tr>
<tr>
<td>D45</td>
<td>-117.3095325</td>
</tr>
<tr>
<td>D46</td>
<td>117.4224534</td>
</tr>
<tr>
<td>D47</td>
<td>-104.0508683</td>
</tr>
<tr>
<td>D48</td>
<td>-63.63811831</td>
</tr>
<tr>
<td>D49</td>
<td>-123.4933319</td>
</tr>
<tr>
<td>D50</td>
<td>-123.6994095</td>
</tr>
<tr>
<td>D51</td>
<td>-27.76330527</td>
</tr>
<tr>
<td>D52</td>
<td>163.5445222</td>
</tr>
<tr>
<td>D53</td>
<td>-126.5386452</td>
</tr>
<tr>
<td>D54</td>
<td>66.65338846</td>
</tr>
<tr>
<td>D55</td>
<td>123.0870013</td>
</tr>
<tr>
<td>D56</td>
<td>103.9181161</td>
</tr>
</tbody>
</table>
CH₂(ads)

Si
Si 1  B1
Si 1  B2  2  A1
Si 2  B3  1  A2  3  D1
Si 2  B4  1  A3  3  D2
Si 5  B5  2  A4  1  D3
Si 3  B6  1  A5  6  D4
Si 2  B7  1  A6  3  D5
Si 8  B8  2  A7  1  D6
Si 7  B9  3  A8  1  D7
Si 9  B10  8  A9  2  D8
Si 3  B11  1  A10  6  D9
C  6  B12  5  A11  2  D10
C  1  B13  3  A12  4  D11
C  2  B14  1  A13  14  D12
C 12  B15  3  A14  1  D13
C 11  B16  9  A15  8  D14
C 10  B17  7  A16  3  D15
C  7  B18  3  A17  1  D16
C 12  B19  3  A18  1  D17
C  7  B20  3  A19  1  D18
C  9  B21  8  A20  2  D19
H  1  B22  14  A21  3  D20
H  2  B23  1  A22  14  D21
<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>3</td>
<td>B24</td>
<td>1</td>
<td>A23</td>
<td>14</td>
</tr>
<tr>
<td>H</td>
<td>5</td>
<td>B25</td>
<td>2</td>
<td>A24</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>16</td>
<td>B26</td>
<td>12</td>
<td>A25</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>6</td>
<td>B27</td>
<td>5</td>
<td>A26</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>17</td>
<td>B28</td>
<td>11</td>
<td>A27</td>
<td>9</td>
</tr>
<tr>
<td>H</td>
<td>18</td>
<td>B29</td>
<td>10</td>
<td>A28</td>
<td>7</td>
</tr>
<tr>
<td>H</td>
<td>19</td>
<td>B30</td>
<td>7</td>
<td>A29</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>20</td>
<td>B31</td>
<td>12</td>
<td>A30</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>21</td>
<td>B32</td>
<td>7</td>
<td>A31</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>22</td>
<td>B33</td>
<td>9</td>
<td>A32</td>
<td>8</td>
</tr>
<tr>
<td>C</td>
<td>4</td>
<td>B34</td>
<td>2</td>
<td>A33</td>
<td>1</td>
</tr>
<tr>
<td>C</td>
<td>3</td>
<td>B35</td>
<td>1</td>
<td>A34</td>
<td>14</td>
</tr>
<tr>
<td>Si</td>
<td>20</td>
<td>B36</td>
<td>12</td>
<td>A35</td>
<td>3</td>
</tr>
<tr>
<td>Si</td>
<td>19</td>
<td>B37</td>
<td>7</td>
<td>A36</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>38</td>
<td>B38</td>
<td>19</td>
<td>A37</td>
<td>7</td>
</tr>
<tr>
<td>Si</td>
<td>36</td>
<td>B39</td>
<td>3</td>
<td>A38</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>39</td>
<td>B40</td>
<td>38</td>
<td>A39</td>
<td>19</td>
</tr>
<tr>
<td>H</td>
<td>39</td>
<td>B41</td>
<td>38</td>
<td>A40</td>
<td>19</td>
</tr>
<tr>
<td>H</td>
<td>40</td>
<td>B42</td>
<td>36</td>
<td>A41</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>40</td>
<td>B43</td>
<td>36</td>
<td>A42</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>38</td>
<td>B44</td>
<td>19</td>
<td>A43</td>
<td>7</td>
</tr>
<tr>
<td>H</td>
<td>7</td>
<td>B45</td>
<td>3</td>
<td>A44</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>36</td>
<td>B46</td>
<td>3</td>
<td>A45</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>14</td>
<td>B47</td>
<td>1</td>
<td>A46</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>13</td>
<td>B48</td>
<td>6</td>
<td>A47</td>
<td>5</td>
</tr>
<tr>
<td>H</td>
<td>11</td>
<td>B49</td>
<td>9</td>
<td>A48</td>
<td>8</td>
</tr>
<tr>
<td>C</td>
<td>1</td>
<td>B50</td>
<td>14</td>
<td>A49</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
<td>B51</td>
<td>1</td>
<td>A50</td>
<td>14</td>
</tr>
<tr>
<td>C</td>
<td>3</td>
<td>B52</td>
<td>1</td>
<td>A51</td>
<td>14</td>
</tr>
<tr>
<td>Si</td>
<td>53</td>
<td>B53</td>
<td>3</td>
<td>A52</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>5</td>
<td>B54</td>
<td>2</td>
<td>A53</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>2</td>
<td>B55</td>
<td>1</td>
<td>A54</td>
<td>14</td>
</tr>
<tr>
<td>H</td>
<td>22</td>
<td>B56</td>
<td>9</td>
<td>A55</td>
<td>8</td>
</tr>
<tr>
<td>H</td>
<td>17</td>
<td>B57</td>
<td>11</td>
<td>A56</td>
<td>9</td>
</tr>
<tr>
<td>H</td>
<td>21</td>
<td>B58</td>
<td>7</td>
<td>A57</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>18</td>
<td>B59</td>
<td>10</td>
<td>A58</td>
<td>7</td>
</tr>
<tr>
<td>H</td>
<td>6</td>
<td>B60</td>
<td>5</td>
<td>A59</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>1</td>
<td>B61</td>
<td>14</td>
<td>A60</td>
<td>3</td>
</tr>
<tr>
<td>Si</td>
<td>15</td>
<td>B62</td>
<td>2</td>
<td>A61</td>
<td>1</td>
</tr>
<tr>
<td>Si</td>
<td>35</td>
<td>B63</td>
<td>4</td>
<td>A62</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>37</td>
<td>B64</td>
<td>20</td>
<td>A63</td>
<td>12</td>
</tr>
<tr>
<td>C</td>
<td>8</td>
<td>B65</td>
<td>2</td>
<td>A64</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>B66</td>
<td>15</td>
<td>A65</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>B67</td>
<td>35</td>
<td>A66</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>B68</td>
<td>35</td>
<td>A67</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>B69</td>
<td>15</td>
<td>A68</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>64</td>
<td>B70</td>
<td>35</td>
<td>A69</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>B71</td>
<td>37</td>
<td>A70</td>
<td>20</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>B72</td>
<td>37</td>
<td>A71</td>
<td>20</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>B73</td>
<td>8</td>
<td>A72</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>B74</td>
<td>8</td>
<td>A73</td>
<td>2</td>
</tr>
<tr>
<td>Si</td>
<td>66</td>
<td>B75</td>
<td>8</td>
<td>A74</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>H</td>
<td>76</td>
<td>B76</td>
<td>66</td>
<td>A75</td>
<td>8</td>
</tr>
<tr>
<td>H</td>
<td>71</td>
<td>B77</td>
<td>64</td>
<td>A76</td>
<td>35</td>
</tr>
<tr>
<td>C</td>
<td>4</td>
<td>B78</td>
<td>2</td>
<td>A77</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>B79</td>
<td>4</td>
<td>A78</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>B80</td>
<td>4</td>
<td>A79</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>54</td>
<td>B81</td>
<td>53</td>
<td>A80</td>
<td>3</td>
</tr>
</tbody>
</table>

<p>| B1 | 6.22824254 |
| B2 | 3.12490123 |
| B3 | 3.11769344 |
| B4 | 3.12555538 |
| B5 | 3.11415772 |
| B6 | 3.15353153 |
| B7 | 3.15295864 |
| B8 | 3.15522111 |
| B9 | 3.14998184 |
| B10| 3.15472409 |
| B11| 3.13836119 |
| B12| 1.9085515  |
| B13| 1.90510444 |
| B14| 1.90982966 |
| B15| 1.91019619 |
| B16| 1.90539133 |
| B17| 1.90657123 |
| B18| 1.9096806  |
| B19| 1.90777412 |
| B20| 1.90354238 |
| B21| 1.89963673 |
| B22| 1.4897187  |
| B23| 1.4885418  |
| B24| 1.49023158 |
| B25| 1.48931876 |
| B26| 1.10471142 |
| B27| 1.48940192 |
| B28| 1.10076809 |
| B29| 1.1007567  |
| B30| 1.10294982 |
| B31| 1.10460165 |
| B32| 1.10052632 |
| B33| 1.10098491 |
| B34| 1.93481672 |
| B35| 1.91026996 |
| B36| 1.9128069  |
| B37| 1.91023303 |
| B38| 1.90285581 |
| B39| 1.90681209 |
| B40| 1.09914228 |
| B41| 1.10058363 |
| B42| 1.49113467 |
| B43| 1.48805051 |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>B44</td>
<td>1.49201457</td>
<td></td>
</tr>
<tr>
<td>B45</td>
<td>1.49200453</td>
<td></td>
</tr>
<tr>
<td>B46</td>
<td>1.10124273</td>
<td></td>
</tr>
<tr>
<td>B47</td>
<td>1.10123652</td>
<td></td>
</tr>
<tr>
<td>B48</td>
<td>1.10075443</td>
<td></td>
</tr>
<tr>
<td>B49</td>
<td>1.49153045</td>
<td></td>
</tr>
<tr>
<td>B50</td>
<td>1.91061018</td>
<td></td>
</tr>
<tr>
<td>B51</td>
<td>1.91013231</td>
<td></td>
</tr>
<tr>
<td>B52</td>
<td>1.91833739</td>
<td></td>
</tr>
<tr>
<td>B53</td>
<td>1.9136359</td>
<td></td>
</tr>
<tr>
<td>B54</td>
<td>1.49042434</td>
<td></td>
</tr>
<tr>
<td>B55</td>
<td>1.49149626</td>
<td></td>
</tr>
<tr>
<td>B56</td>
<td>1.09925739</td>
<td></td>
</tr>
<tr>
<td>B57</td>
<td>1.09906132</td>
<td></td>
</tr>
<tr>
<td>B58</td>
<td>1.09942028</td>
<td></td>
</tr>
<tr>
<td>B59</td>
<td>1.09907853</td>
<td></td>
</tr>
<tr>
<td>B60</td>
<td>1.49046218</td>
<td></td>
</tr>
<tr>
<td>B61</td>
<td>1.49077471</td>
<td></td>
</tr>
<tr>
<td>B62</td>
<td>1.91107839</td>
<td></td>
</tr>
<tr>
<td>B63</td>
<td>1.91121531</td>
<td></td>
</tr>
<tr>
<td>B64</td>
<td>1.90727209</td>
<td></td>
</tr>
<tr>
<td>B65</td>
<td>1.90624271</td>
<td></td>
</tr>
<tr>
<td>B66</td>
<td>1.48849438</td>
<td></td>
</tr>
<tr>
<td>B67</td>
<td>1.49022568</td>
<td></td>
</tr>
<tr>
<td>B68</td>
<td>1.48888723</td>
<td></td>
</tr>
<tr>
<td>B69</td>
<td>1.49049944</td>
<td></td>
</tr>
<tr>
<td>B70</td>
<td>1.9084041</td>
<td></td>
</tr>
<tr>
<td>B71</td>
<td>1.1007758</td>
<td></td>
</tr>
<tr>
<td>B72</td>
<td>1.09885603</td>
<td></td>
</tr>
<tr>
<td>B73</td>
<td>1.10080256</td>
<td></td>
</tr>
<tr>
<td>B74</td>
<td>1.09889069</td>
<td></td>
</tr>
<tr>
<td>B75</td>
<td>1.90439814</td>
<td></td>
</tr>
<tr>
<td>B76</td>
<td>1.49151902</td>
<td></td>
</tr>
<tr>
<td>B77</td>
<td>1.10080647</td>
<td></td>
</tr>
<tr>
<td>B78</td>
<td>1.86766338</td>
<td></td>
</tr>
<tr>
<td>B79</td>
<td>1.0898424</td>
<td></td>
</tr>
<tr>
<td>B80</td>
<td>1.08975628</td>
<td></td>
</tr>
<tr>
<td>B81</td>
<td>1.49144874</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>60.25623618</td>
<td></td>
</tr>
<tr>
<td>A2</td>
<td>60.32473907</td>
<td></td>
</tr>
<tr>
<td>A3</td>
<td>60.11405267</td>
<td></td>
</tr>
<tr>
<td>A4</td>
<td>119.8942606</td>
<td></td>
</tr>
<tr>
<td>A5</td>
<td>60.64600037</td>
<td></td>
</tr>
<tr>
<td>A6</td>
<td>90.95805095</td>
<td></td>
</tr>
<tr>
<td>A7</td>
<td>60.07339087</td>
<td></td>
</tr>
<tr>
<td>A8</td>
<td>90.20663027</td>
<td></td>
</tr>
<tr>
<td>A9</td>
<td>179.4864505</td>
<td></td>
</tr>
<tr>
<td>A10</td>
<td>90.28431963</td>
<td></td>
</tr>
<tr>
<td>A11</td>
<td>35.35149239</td>
<td></td>
</tr>
<tr>
<td>A12</td>
<td>35.07870747</td>
<td></td>
</tr>
<tr>
<td>A13</td>
<td>91.14325574</td>
<td></td>
</tr>
<tr>
<td>A14</td>
<td>121.3768814</td>
<td></td>
</tr>
<tr>
<td>A15</td>
<td>34.12974338</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>A16</td>
<td>146.5961692</td>
<td></td>
</tr>
<tr>
<td>A17</td>
<td>72.53361681</td>
<td></td>
</tr>
<tr>
<td>A18</td>
<td>121.3653066</td>
<td></td>
</tr>
<tr>
<td>A19</td>
<td>122.8975723</td>
<td></td>
</tr>
<tr>
<td>A20</td>
<td>33.89266089</td>
<td></td>
</tr>
<tr>
<td>A21</td>
<td>110.2349437</td>
<td></td>
</tr>
<tr>
<td>A22</td>
<td>89.43264307</td>
<td></td>
</tr>
<tr>
<td>A23</td>
<td>88.96275535</td>
<td></td>
</tr>
<tr>
<td>A24</td>
<td>90.1387376</td>
<td></td>
</tr>
<tr>
<td>A25</td>
<td>107.3164398</td>
<td></td>
</tr>
<tr>
<td>A26</td>
<td>88.99797365</td>
<td></td>
</tr>
<tr>
<td>A27</td>
<td>109.0399115</td>
<td></td>
</tr>
<tr>
<td>A28</td>
<td>108.2985062</td>
<td></td>
</tr>
<tr>
<td>A29</td>
<td>108.3501745</td>
<td></td>
</tr>
<tr>
<td>A30</td>
<td>107.4092077</td>
<td></td>
</tr>
<tr>
<td>A31</td>
<td>109.169239</td>
<td></td>
</tr>
<tr>
<td>A32</td>
<td>108.5250046</td>
<td></td>
</tr>
<tr>
<td>A33</td>
<td>144.6288625</td>
<td></td>
</tr>
<tr>
<td>A34</td>
<td>146.5929298</td>
<td></td>
</tr>
<tr>
<td>A35</td>
<td>111.6990655</td>
<td></td>
</tr>
<tr>
<td>A36</td>
<td>111.6360279</td>
<td></td>
</tr>
<tr>
<td>A37</td>
<td>108.3498087</td>
<td></td>
</tr>
<tr>
<td>A38</td>
<td>110.6662882</td>
<td></td>
</tr>
<tr>
<td>A39</td>
<td>110.6181862</td>
<td></td>
</tr>
<tr>
<td>A40</td>
<td>109.1486623</td>
<td></td>
</tr>
<tr>
<td>A41</td>
<td>110.3448199</td>
<td></td>
</tr>
<tr>
<td>A42</td>
<td>110.5075514</td>
<td></td>
</tr>
<tr>
<td>A43</td>
<td>110.405434</td>
<td></td>
</tr>
<tr>
<td>A44</td>
<td>121.8876337</td>
<td></td>
</tr>
<tr>
<td>A45</td>
<td>107.6556664</td>
<td></td>
</tr>
<tr>
<td>A46</td>
<td>108.0890257</td>
<td></td>
</tr>
<tr>
<td>A47</td>
<td>108.1034335</td>
<td></td>
</tr>
<tr>
<td>A48</td>
<td>145.4587915</td>
<td></td>
</tr>
<tr>
<td>A49</td>
<td>108.5585803</td>
<td></td>
</tr>
<tr>
<td>A50</td>
<td>36.4564291</td>
<td></td>
</tr>
<tr>
<td>A51</td>
<td>89.82895668</td>
<td></td>
</tr>
<tr>
<td>A52</td>
<td>110.1555727</td>
<td></td>
</tr>
<tr>
<td>A53</td>
<td>90.32495957</td>
<td></td>
</tr>
<tr>
<td>A54</td>
<td>145.9290576</td>
<td></td>
</tr>
<tr>
<td>A55</td>
<td>110.4217715</td>
<td></td>
</tr>
<tr>
<td>A56</td>
<td>110.978897</td>
<td></td>
</tr>
<tr>
<td>A57</td>
<td>110.5109637</td>
<td></td>
</tr>
<tr>
<td>A58</td>
<td>109.9487373</td>
<td></td>
</tr>
<tr>
<td>A59</td>
<td>145.9153887</td>
<td></td>
</tr>
<tr>
<td>A60</td>
<td>110.7620286</td>
<td></td>
</tr>
<tr>
<td>A61</td>
<td>110.0097861</td>
<td></td>
</tr>
<tr>
<td>A62</td>
<td>109.2623244</td>
<td></td>
</tr>
<tr>
<td>A63</td>
<td>108.5812353</td>
<td></td>
</tr>
<tr>
<td>A64</td>
<td>125.2772693</td>
<td></td>
</tr>
<tr>
<td>A65</td>
<td>110.4658621</td>
<td></td>
</tr>
<tr>
<td>A66</td>
<td>109.9194789</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>A67</td>
<td>110.5484076</td>
<td></td>
</tr>
<tr>
<td>A68</td>
<td>109.9924038</td>
<td></td>
</tr>
<tr>
<td>A69</td>
<td>108.5654476</td>
<td></td>
</tr>
<tr>
<td>A70</td>
<td>108.0832343</td>
<td></td>
</tr>
<tr>
<td>A71</td>
<td>110.046337</td>
<td></td>
</tr>
<tr>
<td>A72</td>
<td>108.1191566</td>
<td></td>
</tr>
<tr>
<td>A73</td>
<td>109.9736165</td>
<td></td>
</tr>
<tr>
<td>A74</td>
<td>111.714168</td>
<td></td>
</tr>
<tr>
<td>A75</td>
<td>111.5267518</td>
<td></td>
</tr>
<tr>
<td>A76</td>
<td>108.0462181</td>
<td></td>
</tr>
<tr>
<td>A77</td>
<td>90.23301704</td>
<td></td>
</tr>
<tr>
<td>A78</td>
<td>122.0972651</td>
<td></td>
</tr>
<tr>
<td>A79</td>
<td>122.7855673</td>
<td></td>
</tr>
<tr>
<td>A80</td>
<td>109.5382584</td>
<td></td>
</tr>
<tr>
<td>D1</td>
<td>0.39291695</td>
<td></td>
</tr>
<tr>
<td>D2</td>
<td>-179.6768661</td>
<td></td>
</tr>
<tr>
<td>D3</td>
<td>0.13656947</td>
<td></td>
</tr>
<tr>
<td>D4</td>
<td>109.3723906</td>
<td></td>
</tr>
<tr>
<td>D5</td>
<td>-54.67483828</td>
<td></td>
</tr>
<tr>
<td>D6</td>
<td>-55.34938723</td>
<td></td>
</tr>
<tr>
<td>D7</td>
<td>-54.40525896</td>
<td></td>
</tr>
<tr>
<td>D8</td>
<td>27.79525413</td>
<td></td>
</tr>
<tr>
<td>D9</td>
<td>54.52863435</td>
<td></td>
</tr>
<tr>
<td>D10</td>
<td>142.3873464</td>
<td></td>
</tr>
<tr>
<td>D11</td>
<td>-143.0649499</td>
<td></td>
</tr>
<tr>
<td>D12</td>
<td>1.03929034</td>
<td></td>
</tr>
<tr>
<td>D13</td>
<td>-14.00009144</td>
<td></td>
</tr>
<tr>
<td>D14</td>
<td>-137.5440625</td>
<td></td>
</tr>
<tr>
<td>D15</td>
<td>163.0759129</td>
<td></td>
</tr>
<tr>
<td>D16</td>
<td>-144.91426</td>
<td></td>
</tr>
<tr>
<td>D17</td>
<td>-164.6077111</td>
<td></td>
</tr>
<tr>
<td>D18</td>
<td>-43.8056561</td>
<td></td>
</tr>
<tr>
<td>D19</td>
<td>-109.9990011</td>
<td></td>
</tr>
<tr>
<td>D20</td>
<td>56.55843914</td>
<td></td>
</tr>
<tr>
<td>D21</td>
<td>111.0391832</td>
<td></td>
</tr>
<tr>
<td>D22</td>
<td>126.714826</td>
<td></td>
</tr>
<tr>
<td>D23</td>
<td>-88.9061264</td>
<td></td>
</tr>
<tr>
<td>D24</td>
<td>144.1720466</td>
<td></td>
</tr>
<tr>
<td>D25</td>
<td>-89.4873785</td>
<td></td>
</tr>
<tr>
<td>D26</td>
<td>-119.6625984</td>
<td></td>
</tr>
<tr>
<td>D27</td>
<td>60.34366479</td>
<td></td>
</tr>
<tr>
<td>D28</td>
<td>179.1075166</td>
<td></td>
</tr>
<tr>
<td>D29</td>
<td>-144.1265996</td>
<td></td>
</tr>
<tr>
<td>D30</td>
<td>-138.8425328</td>
<td></td>
</tr>
<tr>
<td>D31</td>
<td>-119.7031241</td>
<td></td>
</tr>
<tr>
<td>D32</td>
<td>-145.4905877</td>
<td></td>
</tr>
<tr>
<td>D33</td>
<td>0.86713334</td>
<td></td>
</tr>
<tr>
<td>D34</td>
<td>-27.00055431</td>
<td></td>
</tr>
<tr>
<td>D35</td>
<td>-61.7431882</td>
<td></td>
</tr>
<tr>
<td>D36</td>
<td>-178.4659255</td>
<td></td>
</tr>
<tr>
<td>D37</td>
<td>179.2012896</td>
<td></td>
</tr>
<tr>
<td>D38</td>
<td>174.8928679</td>
<td></td>
</tr>
</tbody>
</table>
C$_2$H$_4$(ads)

Si
Si 1 B1
Si 1 B2 2 A1
Si 3 B3 1 A2 2 D1
Si 2 B4 1 A3 3 D2
Si 5 B5 2 A4 1 D3
Si 3 B6 1 A5 6 D4
Si 2 B7 1 A6 3 D5
<p>| Si  | 2   | B8  | 1   | A7  | 3   | D6  |
| Si  | 1   | B9  | 3   | A8  | 4   | D7  |
| Si  | 10  | B10 | 1   | A9  | 3   | D8  |
| Si  | 7   | B11 | 3   | A10 | 1   | D9  |
| C   | 5   | B12 | 2   | A11 | 1   | D10 |
| C   | 3   | B13 | 1   | A12 | 6   | D11 |
| C   | 2   | B14 | 1   | A13 | 14  | D12 |
| C   | 12  | B15 | 7   | A14 | 3   | D13 |
| C   | 9   | B16 | 2   | A15 | 1   | D14 |
| C   | 11  | B17 | 10  | A16 | 1   | D15 |
| C   | 7   | B18 | 3   | A17 | 1   | D16 |
| C   | 12  | B19 | 7   | A18 | 3   | D17 |
| C   | 7   | B20 | 3   | A19 | 1   | D18 |
| C   | 8   | B21 | 2   | A20 | 1   | D19 |
| H   | 1   | B22 | 14  | A21 | 3   | D20 |
| H   | 2   | B23 | 1   | A22 | 14  | D21 |
| H   | 3   | B24 | 1   | A23 | 14  | D22 |
| H   | 5   | B25 | 2   | A24 | 1   | D23 |
| H   | 16  | B26 | 12  | A25 | 7   | D24 |
| H   | 6   | B27 | 5   | A26 | 2   | D25 |
| H   | 17  | B28 | 9   | A27 | 2   | D26 |
| H   | 18  | B29 | 11  | A28 | 10  | D27 |
| H   | 19  | B30 | 7   | A29 | 3   | D28 |
| H   | 20  | B31 | 12  | A30 | 7   | D29 |
| H   | 21  | B32 | 7   | A31 | 3   | D30 |
| H   | 22  | B33 | 8   | A32 | 2   | D31 |
| C   | 4   | B34 | 3   | A33 | 1   | D32 |
| C   | 3   | B35 | 1   | A34 | 14  | D33 |
| Si  | 20  | B36 | 12  | A35 | 7   | D34 |
| Si  | 19  | B37 | 7   | A36 | 3   | D35 |
| C   | 38  | B38 | 19  | A37 | 7   | D36 |
| Si  | 36  | B39 | 3   | A38 | 1   | D37 |
| H   | 39  | B40 | 38  | A39 | 19  | D38 |
| H   | 39  | B41 | 38  | A40 | 19  | D39 |
| H   | 40  | B42 | 36  | A41 | 3   | D40 |
| H   | 40  | B43 | 36  | A42 | 3   | D41 |
| H   | 38  | B44 | 19  | A43 | 7   | D42 |
| H   | 7   | B45 | 3   | A44 | 1   | D43 |
| H   | 36  | B46 | 3   | A45 | 1   | D44 |
| H   | 14  | B47 | 3   | A46 | 1   | D45 |
| H   | 13  | B48 | 5   | A47 | 2   | D46 |
| H   | 11  | B49 | 10  | A48 | 1   | D47 |
| C   | 6   | B50 | 5   | A49 | 2   | D48 |
| C   | 2   | B51 | 1   | A50 | 14  | D49 |
| C   | 12  | B52 | 7   | A51 | 3   | D50 |
| Si  | 53  | B53 | 12  | A52 | 7   | D51 |
| H   | 5   | B54 | 2   | A53 | 1   | D52 |
| H   | 2   | B55 | 1   | A54 | 14  | D53 |
| H   | 22  | B56 | 8   | A55 | 2   | D54 |
| H   | 17  | B57 | 9   | A56 | 2   | D55 |
| H   | 21  | B58 | 7   | A57 | 3   | D56 |
| H   | 18  | B59 | 11  | A58 | 10  | D57 |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>6</td>
<td>B60</td>
<td>5</td>
<td>A59</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>1</td>
<td>B61</td>
<td>14</td>
<td>A60</td>
<td>3</td>
</tr>
<tr>
<td>Si</td>
<td>15</td>
<td>B62</td>
<td>2</td>
<td>A61</td>
<td>1</td>
</tr>
<tr>
<td>Si</td>
<td>35</td>
<td>B63</td>
<td>4</td>
<td>A62</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>37</td>
<td>B64</td>
<td>20</td>
<td>A63</td>
<td>12</td>
</tr>
<tr>
<td>C</td>
<td>8</td>
<td>B65</td>
<td>2</td>
<td>A64</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>B66</td>
<td>15</td>
<td>A65</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>B67</td>
<td>35</td>
<td>A66</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>64</td>
<td>B68</td>
<td>35</td>
<td>A67</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>63</td>
<td>B69</td>
<td>15</td>
<td>A68</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>63</td>
<td>B70</td>
<td>15</td>
<td>A69</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>B71</td>
<td>37</td>
<td>A70</td>
<td>20</td>
</tr>
<tr>
<td>H</td>
<td>65</td>
<td>B72</td>
<td>37</td>
<td>A71</td>
<td>20</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>B73</td>
<td>8</td>
<td>A72</td>
<td>2</td>
</tr>
<tr>
<td>H</td>
<td>66</td>
<td>B74</td>
<td>8</td>
<td>A73</td>
<td>2</td>
</tr>
<tr>
<td>Si</td>
<td>65</td>
<td>B75</td>
<td>37</td>
<td>A74</td>
<td>20</td>
</tr>
<tr>
<td>H</td>
<td>76</td>
<td>B76</td>
<td>65</td>
<td>A75</td>
<td>37</td>
</tr>
<tr>
<td>H</td>
<td>76</td>
<td>B77</td>
<td>63</td>
<td>A76</td>
<td>15</td>
</tr>
<tr>
<td>C</td>
<td>79</td>
<td>B78</td>
<td>3</td>
<td>A77</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>B79</td>
<td>4</td>
<td>A78</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>79</td>
<td>B80</td>
<td>4</td>
<td>A79</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>79</td>
<td>B81</td>
<td>4</td>
<td>A80</td>
<td>3</td>
</tr>
<tr>
<td>H</td>
<td>82</td>
<td>B82</td>
<td>79</td>
<td>A81</td>
<td>4</td>
</tr>
<tr>
<td>H</td>
<td>82</td>
<td>B83</td>
<td>79</td>
<td>A82</td>
<td>4</td>
</tr>
</tbody>
</table>

B1  6.28553347
B2  3.08509068
B3  3.10689486
B4  3.08441276
B5  3.08847244
B6  3.12044014
B7  3.12099573
B8  3.12084203
B9  3.13796728
B10  3.15294888
B11  3.14489532
B12  1.90271594
B13  1.8994673
B14  1.90054965
B15  1.91266803
B16  1.90716515
B17  1.90197548
B18  1.91993913
B19  1.91268726
B20  1.89942637
B21  1.90641881
B22  1.49038285
B23  1.4875188
B24  1.48838833
B25  1.49065923
B26  1.10448565
B27  1.49059692
B28  1.10081199
B29  1.10061632
B30  1.10295934
B31  1.10488868
B32  1.10049639
B33  1.10122723
B34  1.93585541
B35  1.89952319
B36  1.91539683
B37  1.91995262
B38  1.89940439
B39  1.90632586
B40  1.09929996
B41  1.10048939
B42  1.4906975
B43  1.49037689
B44  1.49207792
B45  1.49207416
B46  1.10089218
B47  1.10088879
B48  1.10047354
B49  1.49160413
B50  1.90985335
B51  1.90052579
B52  1.89568095
B53  1.89934357
B54  1.49071577
B55  1.49090007
B56  1.09859314
B57  1.09935285
B58  1.09929926
B59  1.09902058
B60  1.49056309
B61  1.4906972
B62  1.90736279
B63  1.90987865
B64  1.90652512
B65  1.90712925
B66  1.49066359
B67  1.4905672
B68  1.49059413
B69  1.49070745
B70  1.90269524
B71  1.10061192
B72  1.0990237
B73  1.10082009
B74  1.09934944
B75  1.9019373
B76  1.49160397
B77  1.10047261
B78  1.93598368
<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>B79</td>
<td>1.09654781</td>
</tr>
<tr>
<td>B80</td>
<td>1.09705371</td>
</tr>
<tr>
<td>B81</td>
<td>1.598451</td>
</tr>
<tr>
<td>B82</td>
<td>1.09700894</td>
</tr>
<tr>
<td>B83</td>
<td>1.09658177</td>
</tr>
<tr>
<td>A1</td>
<td>61.12125515</td>
</tr>
<tr>
<td>A2</td>
<td>117.4049416</td>
</tr>
<tr>
<td>A3</td>
<td>59.29713265</td>
</tr>
<tr>
<td>A4</td>
<td>121.3038093</td>
</tr>
<tr>
<td>A5</td>
<td>62.12431452</td>
</tr>
<tr>
<td>A6</td>
<td>90.2000645</td>
</tr>
<tr>
<td>A7</td>
<td>60.42576974</td>
</tr>
<tr>
<td>A8</td>
<td>89.36034864</td>
</tr>
<tr>
<td>A9</td>
<td>120.1736587</td>
</tr>
<tr>
<td>A10</td>
<td>60.33328721</td>
</tr>
<tr>
<td>A11</td>
<td>144.4988879</td>
</tr>
<tr>
<td>A12</td>
<td>35.91565476</td>
</tr>
<tr>
<td>A13</td>
<td>88.51162086</td>
</tr>
<tr>
<td>A14</td>
<td>89.80051179</td>
</tr>
<tr>
<td>A15</td>
<td>123.1846124</td>
</tr>
<tr>
<td>A16</td>
<td>34.16408498</td>
</tr>
<tr>
<td>A17</td>
<td>72.92142576</td>
</tr>
<tr>
<td>A18</td>
<td>147.3964345</td>
</tr>
<tr>
<td>A19</td>
<td>120.9572109</td>
</tr>
<tr>
<td>A20</td>
<td>75.09340896</td>
</tr>
<tr>
<td>A21</td>
<td>109.7238189</td>
</tr>
<tr>
<td>A22</td>
<td>94.06277021</td>
</tr>
<tr>
<td>A23</td>
<td>87.22765077</td>
</tr>
<tr>
<td>A24</td>
<td>90.63330022</td>
</tr>
<tr>
<td>A25</td>
<td>108.9925612</td>
</tr>
<tr>
<td>A26</td>
<td>88.62620418</td>
</tr>
<tr>
<td>A27</td>
<td>108.744977</td>
</tr>
<tr>
<td>A28</td>
<td>109.3973352</td>
</tr>
<tr>
<td>A29</td>
<td>108.003202</td>
</tr>
<tr>
<td>A30</td>
<td>108.9875099</td>
</tr>
<tr>
<td>A31</td>
<td>110.0257245</td>
</tr>
<tr>
<td>A32</td>
<td>108.0154068</td>
</tr>
<tr>
<td>A33</td>
<td>88.85952786</td>
</tr>
<tr>
<td>A34</td>
<td>148.1030884</td>
</tr>
<tr>
<td>A35</td>
<td>111.2096801</td>
</tr>
<tr>
<td>A36</td>
<td>111.9829495</td>
</tr>
<tr>
<td>A37</td>
<td>109.479807</td>
</tr>
<tr>
<td>A38</td>
<td>108.3027142</td>
</tr>
<tr>
<td>A39</td>
<td>110.1225552</td>
</tr>
<tr>
<td>A40</td>
<td>110.0386807</td>
</tr>
<tr>
<td>A41</td>
<td>111.1434245</td>
</tr>
<tr>
<td>A42</td>
<td>109.7170104</td>
</tr>
<tr>
<td>A43</td>
<td>110.0164651</td>
</tr>
<tr>
<td>A44</td>
<td>122.9738581</td>
</tr>
<tr>
<td>A45</td>
<td>108.1793851</td>
</tr>
<tr>
<td>A46</td>
<td>108.1913719</td>
</tr>
<tr>
<td>A47</td>
<td>108.54835</td>
</tr>
<tr>
<td>Cell</td>
<td>Value</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>A48</td>
<td>145.782868</td>
</tr>
<tr>
<td>A49</td>
<td>90.29724436</td>
</tr>
<tr>
<td>A50</td>
<td>34.58420783</td>
</tr>
<tr>
<td>A51</td>
<td>88.63030973</td>
</tr>
<tr>
<td>A52</td>
<td>113.1805381</td>
</tr>
<tr>
<td>A53</td>
<td>88.55416685</td>
</tr>
<tr>
<td>A54</td>
<td>144.5642326</td>
</tr>
<tr>
<td>A55</td>
<td>110.785171</td>
</tr>
<tr>
<td>A56</td>
<td>109.9220527</td>
</tr>
<tr>
<td>A57</td>
<td>110.1256939</td>
</tr>
<tr>
<td>A58</td>
<td>111.0593342</td>
</tr>
<tr>
<td>A59</td>
<td>146.5989296</td>
</tr>
<tr>
<td>A60</td>
<td>111.1376498</td>
</tr>
<tr>
<td>A61</td>
<td>108.190323</td>
</tr>
<tr>
<td>A62</td>
<td>110.7864756</td>
</tr>
<tr>
<td>A63</td>
<td>108.5872558</td>
</tr>
<tr>
<td>A64</td>
<td>123.181898</td>
</tr>
<tr>
<td>A65</td>
<td>109.7873497</td>
</tr>
<tr>
<td>A66</td>
<td>110.2999638</td>
</tr>
<tr>
<td>A67</td>
<td>109.7964734</td>
</tr>
<tr>
<td>A68</td>
<td>110.1023732</td>
</tr>
<tr>
<td>A69</td>
<td>108.6907752</td>
</tr>
<tr>
<td>A70</td>
<td>107.7301612</td>
</tr>
<tr>
<td>A71</td>
<td>109.9875404</td>
</tr>
<tr>
<td>A72</td>
<td>108.7500396</td>
</tr>
<tr>
<td>A73</td>
<td>109.9246685</td>
</tr>
<tr>
<td>A74</td>
<td>111.7625331</td>
</tr>
<tr>
<td>A75</td>
<td>111.6806228</td>
</tr>
<tr>
<td>A76</td>
<td>108.5567987</td>
</tr>
<tr>
<td>A77</td>
<td>83.28755979</td>
</tr>
<tr>
<td>A78</td>
<td>110.7328916</td>
</tr>
<tr>
<td>A79</td>
<td>110.1427052</td>
</tr>
<tr>
<td>A80</td>
<td>109.9626204</td>
</tr>
<tr>
<td>A81</td>
<td>109.4176879</td>
</tr>
<tr>
<td>A82</td>
<td>109.9503</td>
</tr>
<tr>
<td>D1</td>
<td>-3.01799987</td>
</tr>
<tr>
<td>D2</td>
<td>-179.8662171</td>
</tr>
<tr>
<td>D3</td>
<td>-0.28676284</td>
</tr>
<tr>
<td>D4</td>
<td>109.561139</td>
</tr>
<tr>
<td>D5</td>
<td>-51.38422965</td>
</tr>
<tr>
<td>D6</td>
<td>-107.2730527</td>
</tr>
<tr>
<td>D7</td>
<td>-57.90181824</td>
</tr>
<tr>
<td>D8</td>
<td>126.6489724</td>
</tr>
<tr>
<td>D9</td>
<td>-110.3462529</td>
</tr>
<tr>
<td>D10</td>
<td>38.56403783</td>
</tr>
<tr>
<td>D11</td>
<td>142.3647068</td>
</tr>
<tr>
<td>D12</td>
<td>5.60231754</td>
</tr>
<tr>
<td>D13</td>
<td>125.028997</td>
</tr>
<tr>
<td>D14</td>
<td>-109.979352</td>
</tr>
<tr>
<td>D15</td>
<td>107.5166394</td>
</tr>
<tr>
<td>D16</td>
<td>-146.2003589</td>
</tr>
<tr>
<td>D17</td>
<td>-97.95520358</td>
</tr>
<tr>
<td>Index</td>
<td>Value</td>
</tr>
<tr>
<td>-------</td>
<td>--------------</td>
</tr>
<tr>
<td>D18</td>
<td>-43.34990854</td>
</tr>
<tr>
<td>D19</td>
<td>-88.36752776</td>
</tr>
<tr>
<td>D20</td>
<td>59.15883199</td>
</tr>
<tr>
<td>D21</td>
<td>116.4650965</td>
</tr>
<tr>
<td>D22</td>
<td>127.6830803</td>
</tr>
<tr>
<td>D23</td>
<td>-88.54715351</td>
</tr>
<tr>
<td>D24</td>
<td>88.61004266</td>
</tr>
<tr>
<td>D25</td>
<td>-90.89578597</td>
</tr>
<tr>
<td>D26</td>
<td>-147.3093916</td>
</tr>
<tr>
<td>D27</td>
<td>119.2272711</td>
</tr>
<tr>
<td>D28</td>
<td>-178.8928266</td>
</tr>
<tr>
<td>D29</td>
<td>-64.21115891</td>
</tr>
<tr>
<td>D30</td>
<td>-138.5021264</td>
</tr>
<tr>
<td>D31</td>
<td>175.9428759</td>
</tr>
<tr>
<td>D32</td>
<td>168.0528393</td>
</tr>
<tr>
<td>D33</td>
<td>5.91776412</td>
</tr>
<tr>
<td>D34</td>
<td>52.89027635</td>
</tr>
<tr>
<td>D35</td>
<td>-60.09465354</td>
</tr>
<tr>
<td>D36</td>
<td>177.6083548</td>
</tr>
<tr>
<td>D37</td>
<td>172.8667674</td>
</tr>
<tr>
<td>D38</td>
<td>174.6659158</td>
</tr>
<tr>
<td>D39</td>
<td>57.1955264</td>
</tr>
<tr>
<td>D40</td>
<td>-177.6894097</td>
</tr>
<tr>
<td>D41</td>
<td>-59.16858021</td>
</tr>
<tr>
<td>D42</td>
<td>-59.51990433</td>
</tr>
<tr>
<td>D43</td>
<td>110.6412643</td>
</tr>
<tr>
<td>D44</td>
<td>55.83127963</td>
</tr>
<tr>
<td>D45</td>
<td>117.0540162</td>
</tr>
<tr>
<td>D46</td>
<td>176.900352</td>
</tr>
<tr>
<td>D47</td>
<td>103.2496284</td>
</tr>
<tr>
<td>D48</td>
<td>18.90154931</td>
</tr>
<tr>
<td>D49</td>
<td>-121.7051021</td>
</tr>
<tr>
<td>D50</td>
<td>19.461996</td>
</tr>
<tr>
<td>D51</td>
<td>92.83646958</td>
</tr>
<tr>
<td>D52</td>
<td>164.2068491</td>
</tr>
<tr>
<td>D53</td>
<td>-118.0445864</td>
</tr>
<tr>
<td>D54</td>
<td>-67.35317025</td>
</tr>
<tr>
<td>D55</td>
<td>-30.87558534</td>
</tr>
<tr>
<td>D56</td>
<td>104.0347626</td>
</tr>
<tr>
<td>D57</td>
<td>-123.2486517</td>
</tr>
<tr>
<td>D58</td>
<td>148.5470475</td>
</tr>
<tr>
<td>D59</td>
<td>177.6797151</td>
</tr>
<tr>
<td>D60</td>
<td>146.4827125</td>
</tr>
<tr>
<td>D61</td>
<td>150.6979555</td>
</tr>
<tr>
<td>D62</td>
<td>-177.4505895</td>
</tr>
<tr>
<td>D63</td>
<td>163.1594701</td>
</tr>
<tr>
<td>D64</td>
<td>-61.41513214</td>
</tr>
<tr>
<td>D65</td>
<td>-177.7309498</td>
</tr>
<tr>
<td>D66</td>
<td>-59.50783032</td>
</tr>
<tr>
<td>D67</td>
<td>56.45119309</td>
</tr>
<tr>
<td>D68</td>
<td>178.2725589</td>
</tr>
<tr>
<td>D69</td>
<td>59.23630953</td>
</tr>
<tr>
<td>D70</td>
<td>175.1752528</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
</tr>
<tr>
<td>D71</td>
<td>147.3300074</td>
</tr>
<tr>
<td>D72</td>
<td>30.8935878</td>
</tr>
<tr>
<td>D73</td>
<td>-60.97576617</td>
</tr>
<tr>
<td>D74</td>
<td>-177.4281539</td>
</tr>
<tr>
<td>D75</td>
<td>-178.6728033</td>
</tr>
<tr>
<td>D76</td>
<td>-67.80992227</td>
</tr>
<tr>
<td>D77</td>
<td>-175.7144806</td>
</tr>
<tr>
<td>D78</td>
<td>-58.08666371</td>
</tr>
<tr>
<td>D79</td>
<td>62.57122118</td>
</tr>
<tr>
<td>D80</td>
<td>-121.1447772</td>
</tr>
</tbody>
</table>