

## **London Dispersion Directs On-Surface Self-Assembly of [121]Tetramantane Molecules**

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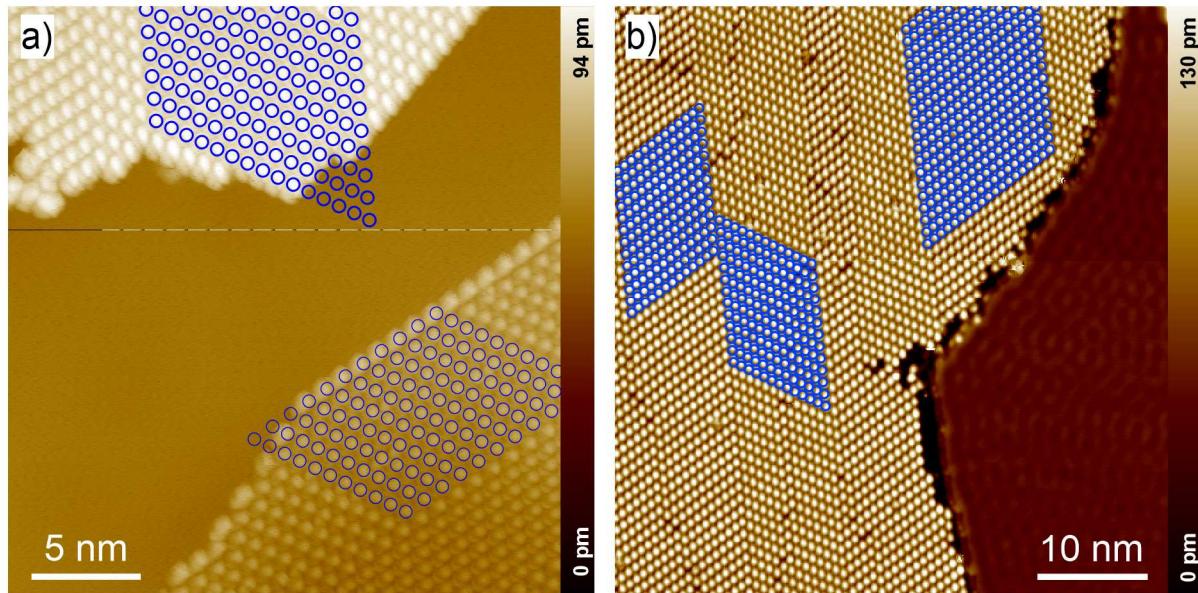
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## STM/AFM measurements

**Figure S1 – Large scale islands of [121]tetramantane on Cu(111).**

Figure S1 shows three different islands of [121]tetramantane (**1**) on a Cu(111) substrate. Regular 2D lattices are fitted to the islands to determine the lattice parameters of the adsorption layer (blue circles). The islands are composed of grains with different orientation but with identical lattice parameters, which correspond to a  $(3 \times 4)$  overlayer structure (in case of Cu(111)).

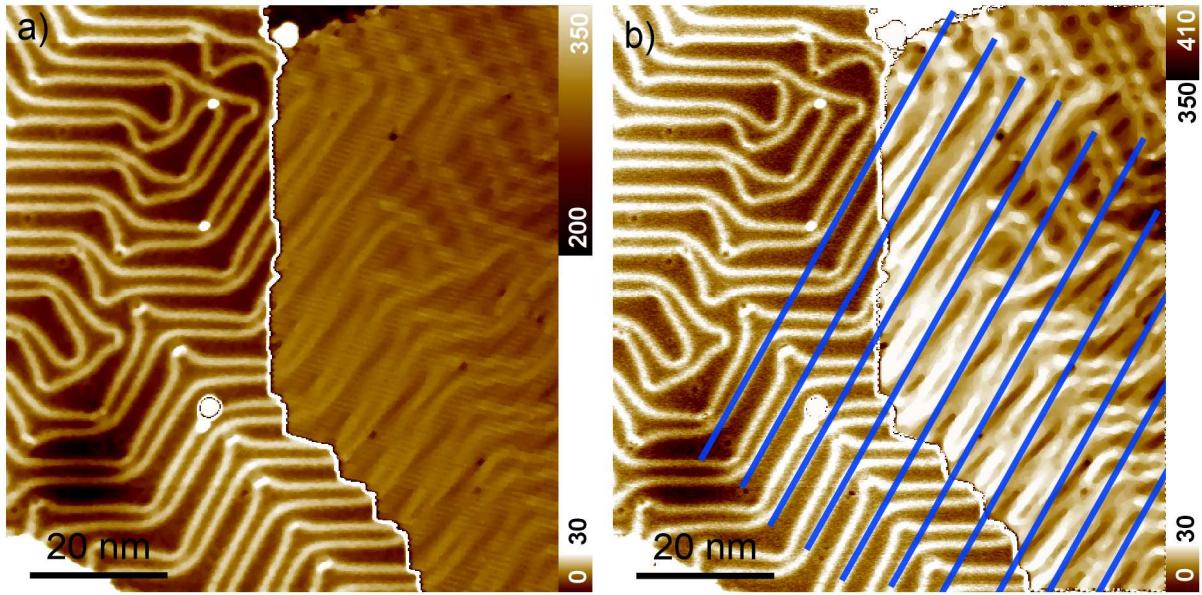


**Figure S1.** Large scale islands of [121]tetramantane on Cu(111). (a), (b) STM images of 2D [121]tetramantane islands on Cu(111) substrate. Blue circles represent a regular 2D lattice with lattice parameters  $\mathbf{a} = (10.2 \pm 0.1) \text{ \AA}$ ,  $\mathbf{b} = (7.7 \pm 0.1) \text{ \AA}$ ,  $\alpha = (60 \pm 1)^\circ$ .

**Figure S2 – Au(111) reconstruction beneath the molecular layer.**

Figure S2a shows the same molecular island as depicted in Figure 1a in the manuscript. To reveal the herringbone reconstruction beneath the molecular layer (right part) more clearly, the image has been convolution filtered and enhanced in contrast (Figure S2b).

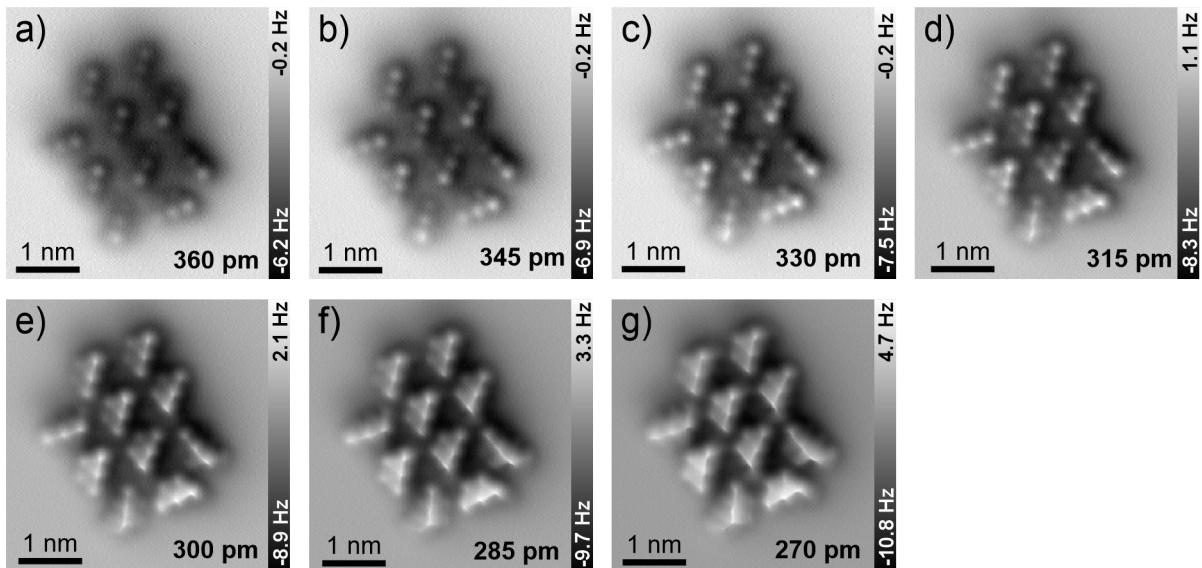
It has been previously observed that the Au(111) herringbone reconstruction is very sensitive to molecular adsorption.<sup>1-3</sup> It was reported that interactions between the Au atoms in the surface plane and the adsorbed molecular species lead to a stress relaxation with the Au surface plane, which results in an elongation of the periodicity of the surface reconstruction. In our case, however, the Au(111) reconstruction is nearly unaffected by the adsorbed molecular layer. This is revealed by the blue lines in Figure S2b, which are oriented along the [11-2] crystallographic direction of the Au(111) surface. The periodicity of the Au(111) reconstruction beneath the molecular layer is virtually unaffected, which indicates remarkably low molecule-substrate interactions.



**Figure S2.** Au(111) reconstruction beneath the molecular layer. (a) STM overview image of large scale 2D island of [121]tetramantane on Au(111). The color scale is split into two parts to reveal the herringbone reconstruction of the Au(111) surface (left part) and the molecular island (right part), side by side. (b) Filtered and contrast enhanced image. Blue lines are orientated along the [11-2]-direction.

### Figure S3 – Series of constant height AFM scans.

Figure S3 shows the full series of constant height AFM scans above the small molecular island presented in Figure 2 in the manuscript. This image series was used to generate a 3D frequency shift map  $\Delta f(x,y,z)$  (Figure S4).



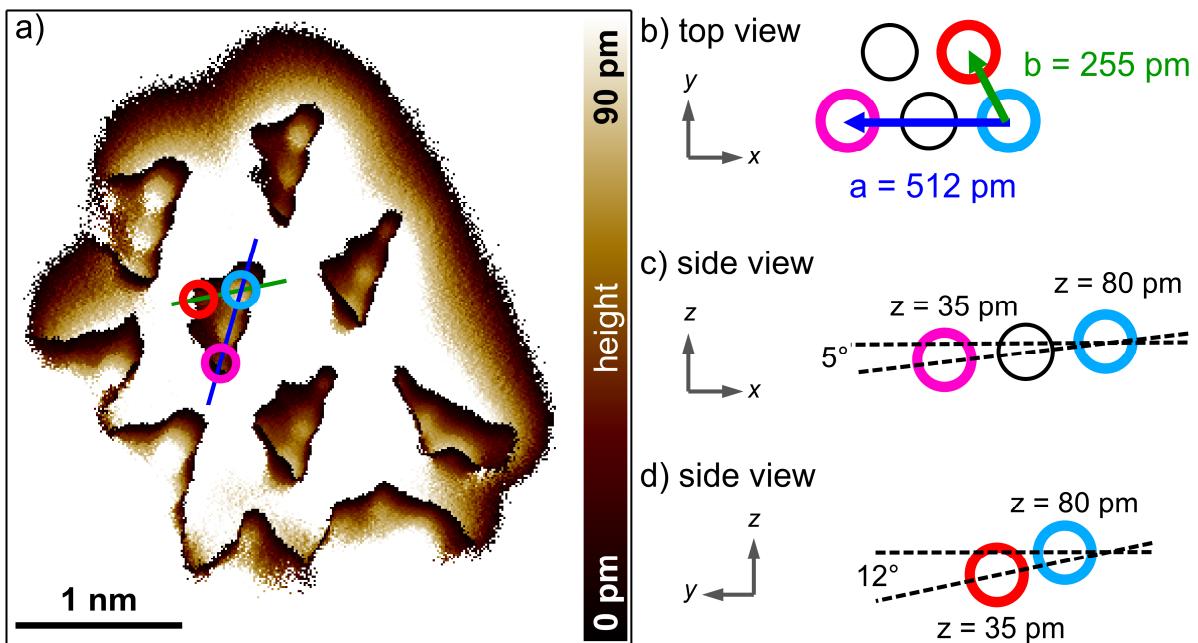
**Figure S3.** Series of constant height AFM scans. (a)-(g) AFM images of a small cluster of [121]tetramantane on Au(111) obtained at seven different imaging heights ranging between  $\Delta z = 360$  and 270 pm (with respect to tunneling gap at 200 mV, 150 pA).

**Figure S4 – Tilting angle of [121]tetramantane on Au(111).**

Figure S4a shows a topography image, which has been calculated from the series of images shown in Figure S3a-g. First, the constant height frequency shift images of the series have been used to generate a 3D frequency shift map  $\Delta f(x,y,z)$ . Since the experimental drift was sufficiently low during the period of the measurement, no additional drift correction was performed. Subsequently, at each pixel of the frequency shift map (*i.e.*, for all  $xy$  coordinates) a height (topography) value was determined by finding the  $z$  position at which a certain frequency shift value ( $-4$  Hz, in this case) is crossed, meaning that for each pixel the  $z$  position was determined, which fulfilled  $\Delta f(z) = -4$  Hz. Therefore, each  $\Delta f(z)$  curve has been linearly interpolated.

The specific frequency shift value of  $-4$  Hz has been chosen, since this frequency level is more positive than the minimum frequency shift in Figure S3a ( $-6$  Hz). This guarantees that the crossing point ( $z$ -value) above the molecules is located well within the repulsive regime of the  $\Delta f(z)$  curve where linear interpolation is reasonable. There are regions in the image, *e.g.*, above the Au surface, where the value of  $-4$  Hz is not crossed. These pixels are displayed in white color.

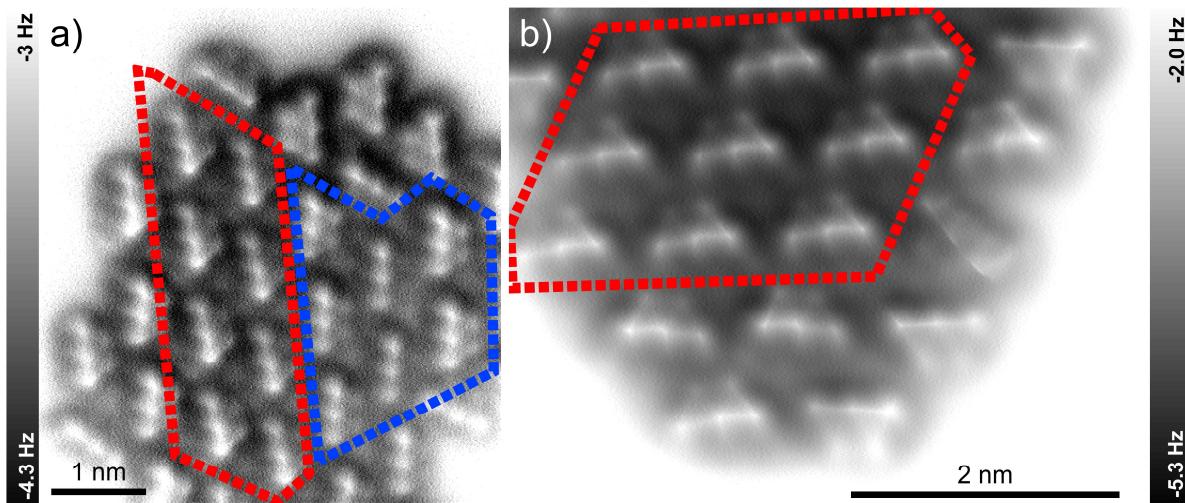
To calculate the tilting angle of the molecules, the height values of certain hydrogen atoms within the five-atom pattern (red, blue, and magenta circles) are determined from the topography image. This analysis reveals a tilting angle of approx.  $5^\circ$  and  $12^\circ$  in  $x$  and  $y$  directions, respectively.



**Figure S4.** Tilting angle of [121]tetramantane on Au(111). (a) Topography image calculated from image series in Figure S3. (b), (c), (d) Top and side views of certain hydrogen atoms within five-atom pattern.

**Figure S5 – Medium sized molecular clusters on Au(111) and Cu(111).**

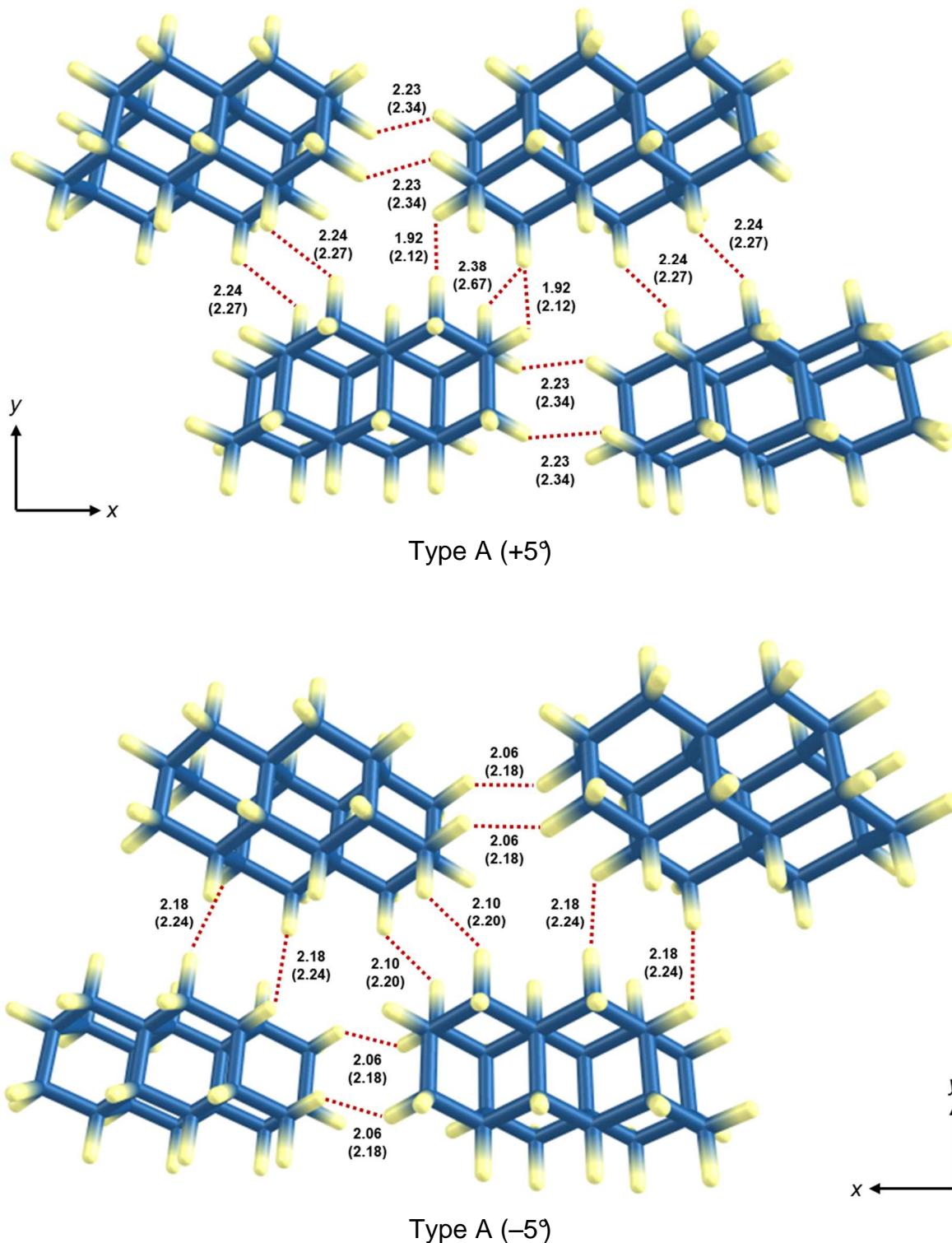
Figure S5 shows two medium sized molecular islands (20–30 molecules) on Au(111) and Cu(111). Clusters with nearly “perfect” molecular arrangement (of 7–9 molecules) are observed within islands (red and blue dashed boxes). The observed clusters correspond to Type A ( $P_{\text{surf}}$ ) (red boxes) and Type A ( $M_{\text{surf}}$ ) (blue box) structures.



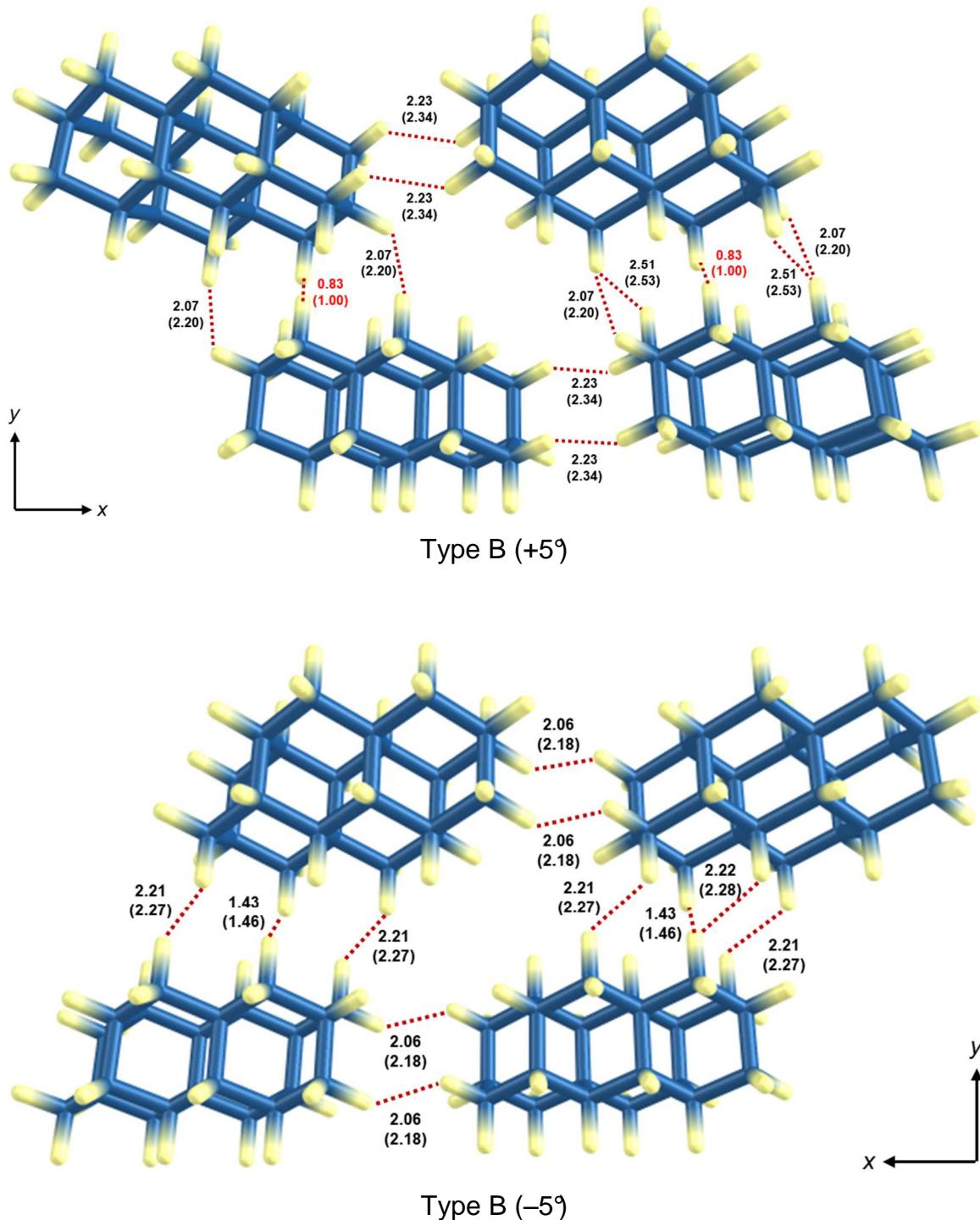
**Figure S5.** Medium sized molecular clusters on Au(111) and Cu(111). (a) AFM frequency shift image of medium size molecular island on Au(111). (b) Medium size island on Cu(111). Clusters with nearly “perfect” molecular arrangement are indicated by red and blue dashed boxes.

**Figures S6-S8 – Structures with  $+5^\circ$  vs.  $-5^\circ$  tilting.**

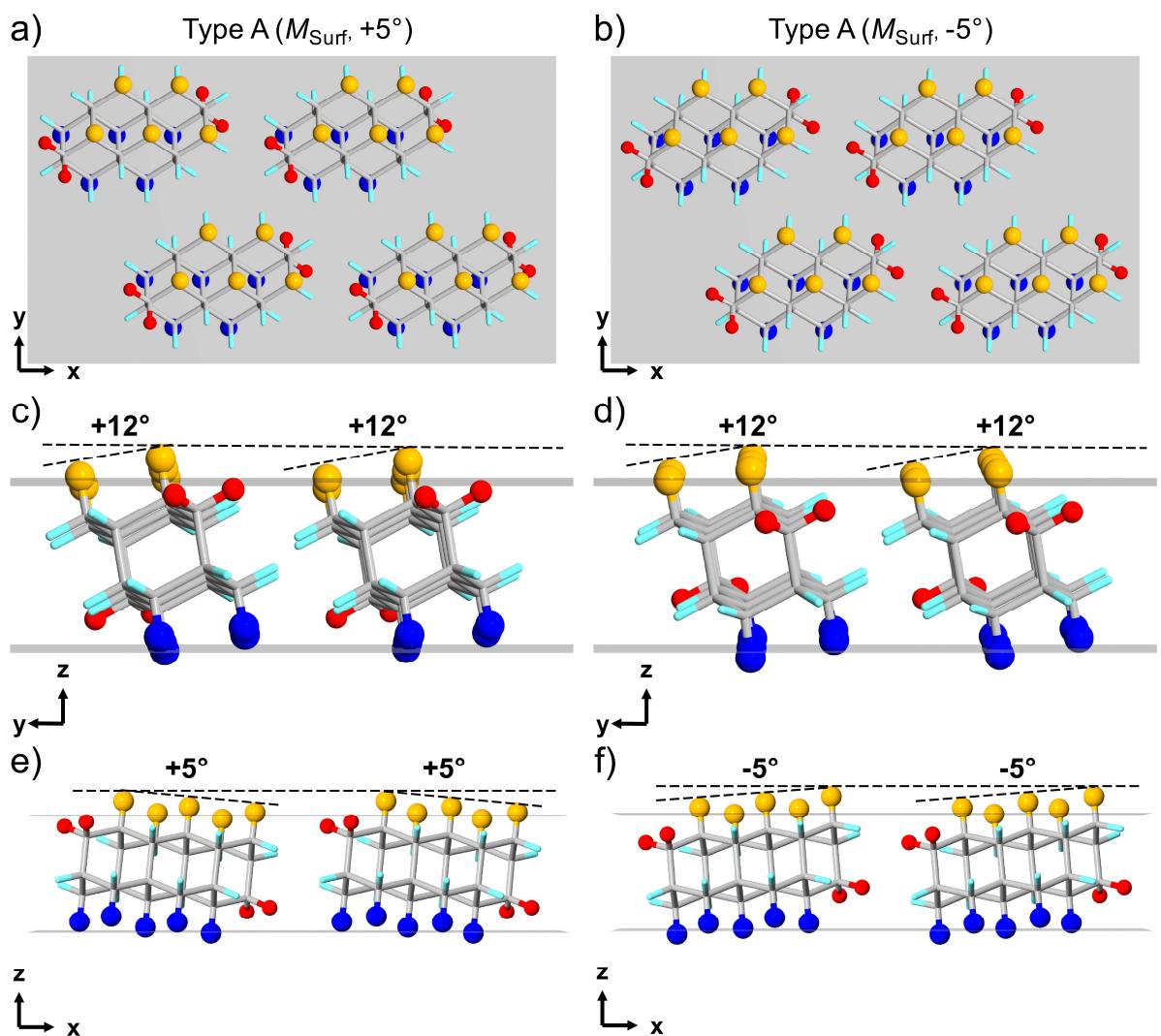
Figure S8 shows two different Type A ( $M_{\text{surf}}$ ) structures, which are either tilted by  $+5^\circ$  (a, c, e) or by  $-5^\circ$  (b, d, f) along the  $x$  direction and figures S6 and S7 show the corresponding computed tetramer structures with highlighted intermolecular close contacts. Using the bond imaging method the five-atom pattern (orange spheres) of the imaged molecules can be identified unambiguously. However, the precise information about the orientation of the five-atom pattern is not sufficient for an absolute identification of molecular orientation as described in the manuscript. Hence, we considered Type A and Type B structures in our analysis (Figure 3 and Table 1 in the manuscript). However, since each molecule within the molecular layer is also tilted with respect to the metal surface plane (Figure 2f, g in the manuscript), one also needs to consider the opposite direction of tilting along the  $x$  direction for each type of structure. Hence, the computations for each structural type (A and B) have been performed for both possible tilting angles, *i.e.*  $+5^\circ$  and  $-5^\circ$ .



**Figure S6.** Structures of the computed type A [121]tetramantane tetramers with different tilting angles on Au(111) surface. Selected H–H distances are given in Å and the values in parenthesis are for the Cu(111) surface. Computations were performed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.



**Figure S7.** Structures of the computed type B [121]tetramantane tetramers with different tilting angles on Au(111) surface. Selected H–H distances are given in Å and the values in parenthesis are for the Cu(111) surface. Computations were performed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.



**Figure S8.** Structures with  $+5^\circ$  vs.  $-5^\circ$  tilting. Type A ( $M_{\text{Surf}}$ ) structure for two different tilting angles along  $x$ -direction. (a), (c), (e)  $+5^\circ$ , (b), (d), (f)  $-5^\circ$ .

## Computation methodology

All geometry optimizations were performed with the GAUSSIAN09 program package<sup>4</sup> by taking the X-ray single-crystal structure of [121]tetramantane (**1**) as a starting point.<sup>5</sup> All structures were optimized using several DFT approaches (B3LYP, B3LYP-D3(BJ), and M06-2X). Verification of the minima by frequency computations was performed and the energies given are corrected for zero-point vibrational energies (ZPVEs). For some structures proper minima could not be obtained, however, the errors are estimated to be minute since the computed imaginary frequencies are quite small (<25 cm<sup>-1</sup>). Single-point energies on the DFT-optimized structures were computed using the ORCA 4.0.0 program<sup>6</sup> at the RI-MP2/cc-pVDZ, RI-MP2/cc-pVTZ, and DLPNO-CCSD(T)/cc-pVDZ levels of theory.

Since the ubiquitous B3LYP functional<sup>7-8</sup> essentially does not include London dispersion (LD),<sup>9-11</sup> it needs to be augmented by a correction such as Grimme's D3-dispersion formulation<sup>12</sup> in connection with Becke-Johnson (BJ) damping to avoid overbinding at short distances.<sup>13-14</sup> This approach allows for an analysis of the LD contribution in the studied [121]tetramantane dimers (**D1–D8**). In addition, we used modern DFT functional M06-2X<sup>15</sup> as well as second order Møller-Plesset perturbation theory MP2,<sup>16</sup> which also describe well the interactions between such hydrocarbons, as shown previously.<sup>17-18</sup> Accurate but very time-consuming single-point interaction energies of the [121]tetramantane dispersion-bound complexes were computed using the highly accurate CCSD(T) *ab initio* method in conjunction with an cc-pVDZ basis set.<sup>19</sup> All RI-MP2<sup>20-23</sup> and DLPNO-CCSD(T)<sup>24-26</sup> single-point computations were performed on optimized geometries obtained by B3LYP-D3(BJ)/6-31G(d,p) level of theory and TightPNO accuracy settings were used for the DLPNO method.

In order to obtain an accurate estimate for the CCSD(T) interaction energies for LD-bound dimers **D1–D8**, we used the complete basis set extrapolation method.<sup>27</sup> This approach partitions the total energy ( $\Delta E_{\text{est}}^{\text{CCSD(T)}}$ ) into the HF energy ( $\Delta E_{\text{CBS}}^{\text{HF}}$ ), the MP2 correlation energy ( $\Delta E_{\text{CBS}}^{\text{MP2,corr}}$ ) and into the contributions of higher order correlation effects [ $\Delta \text{CCSD(T)}$ ] (Eq. 1-5). Since MP2 and CCSD(T) correlation energies converge at a similar rate, it is possible to estimate the CCSD(T)/CBS energy using only moderately sized basis sets.<sup>28</sup>

In our case, for the cc-pVDZ and cc-pVTZ basis sets, the energy ( $\Delta E_{\text{CBS}}^{\text{HF}}$  and  $\Delta E_{\text{CBS}}^{\text{MP2,corr}}$ , respectively) can be expressed as

$$\Delta E_{\text{CBS}}^{\text{HF}} = \frac{3^\alpha}{3^\alpha - 2^\alpha} E_3^{\text{HF}} - \frac{2^\alpha}{3^\alpha - 2^\alpha} E_2^{\text{HF}} \quad \text{Eq. 1}$$

and

$$\Delta E_{\text{CBS}}^{\text{MP2,corr}} = \frac{3^\beta}{3^\beta - 2^\beta} E_3^{\text{MP2,corr}} - \frac{2^\beta}{3^\beta - 2^\beta} E_2^{\text{MP2,corr}} \quad \text{Eq. 2}$$

with the reported optimized exponent values  $\alpha_{23} = 4.42$  and  $\beta_{23} = 2.46$ .<sup>29</sup>

The basis set limit for MP2 is defined as

$$\Delta E_{\text{CBS}}^{\text{MP2}} = \Delta E_{\text{CBS}}^{\text{HF}} + \Delta E_{\text{CBS}}^{\text{MP2,corr}} \quad \text{Eq. 3}$$

and the estimate for the CCSD(T) energies corresponds to

$$\Delta E_{\text{est}}^{\text{CCSD(T)}} = \Delta E_{\text{CBS}}^{\text{MP2}} + \Delta \text{CCSD(T)} \quad \text{Eq. 4}$$

with  $\Delta \text{CCSD(T)}$  equalling to

$$\Delta \text{CCSD(T)} = (E^{\text{CCSD(T)}} - E^{\text{MP2}})_{\text{small basis set}} \quad \text{Eq. 5}$$

Using this procedure we obtained RI-MP2/CBS and DLPNO-CCSD(T)/CBS interaction energies that are presented in Table S1 in parentheses. When adding the corresponding zero-point vibrational energies (ZPVEs) of **1** and **D1–D8** (computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory) to the computed RI-MP2 and DLPNO-CCSD(T) energies,  $\Delta H(0 \text{ K})$  was determined (Table S1).

We studied eight orientations of two [121]tetramantanes (Figure S9). In **D1** both tetramantanes are interacting along the axis with six C–H bonds pointing toward the same direction and therefore engage in most numerous close contacts between the two molecules. This orientation is energetically most favourable, as shown in Table S1. In dimer **D4** a similar interaction is taking place but the contact plane is somewhat shifted to the side and therefore the LD-bound complex is a little lower in energy. Dimers **D2**, **D7**, and **D8** engage in different interactions along the sides of the cages and **D5** combines an axis and side interaction. Although these geometries are LD stabilized somewhat, they cannot capture the full potential of beneficial LD interactions. **D3** is highly unfavourable since it does not

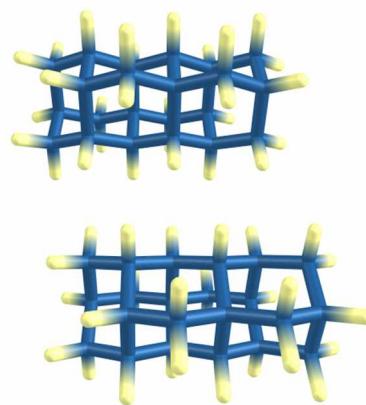
interact along the full length of both cages and has only a limited number of close contacts. This is similarly true for **D6** in which the two tetramantanes are perpendicularly placed forming a T-shaped orientation.

All computation methods (except for the uncorrected B3LYP which does not account for LD and for which dimer starting geometries dissociated during the optimization) showed comparable trends in interaction energies for **D1–D8** (Table S1). The M06-2X approach gave the lowest interaction energies, which can be rationalized by the limitation of the method since it is parametrized for medium-range correlation. For our bulky LD-bound complexes longer-distance correlation obviously plays a part. Energies obtained from B3LYP-D3(BJ)/6-31G(d,p) were in excellent agreement with energies from RI-MP2/cc-pVTZ, confirming the efficacy of the applied D3 correction. However, it is known that MP2 interaction energies sometimes differ from CCSD(T) energies for dispersion-bound complexes.<sup>30</sup> Accordingly, the DLPNO-CCSD(T)/cc-pVDZ level of theory gave somewhat lower energy values while the DLPNO-CCSD(T)/CBS extrapolation data compared well with the RI-MP2 and B3LYP-D3 results. Despite the small differences found between methods, the overall interaction energies for a given LD-bound complex remain comparable, approaching 10 kcal mol<sup>-1</sup> for the most stable dimers.

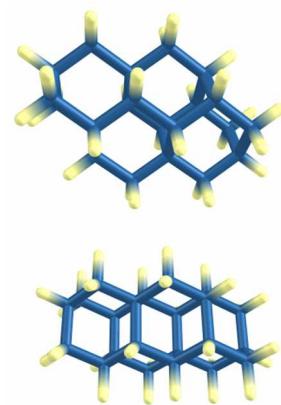
Another validity confirmation of our computational approach comes from Local Energy Decomposition (LED) analysis<sup>31</sup> which is implemented in ORCA 4.0.0 for the DLPNO-CCSD(T) method. In LD-bound complexes **D1–D8** each [121]tetramantane moiety was defined as one fragment and the interaction energy between the two fragments was divided into physically meaningful contributions. Although decomposition of total energies (obtained from DLPNO-CCSD(T)/cc-pVDZ) is in principle arbitrary, the LED analysis is still physically well-grounded and can serve to estimate non-covalent interactions. In our case, decomposition of the CCSD pair energies afforded dispersion contributions that are in agreement with estimates of dispersion energies obtained from other methods shown in Table S1.

In conclusion, we found that **D1** is the energetically most stable dimer from the studied series of LD-bound complexes. In this geometry the number of close contacts between tetramantanes is maximised, confirming that LD is an important interaction for aggregate formation and that it is responsible for the preferred orientation of the molecules on essentially non-interacting surfaces.

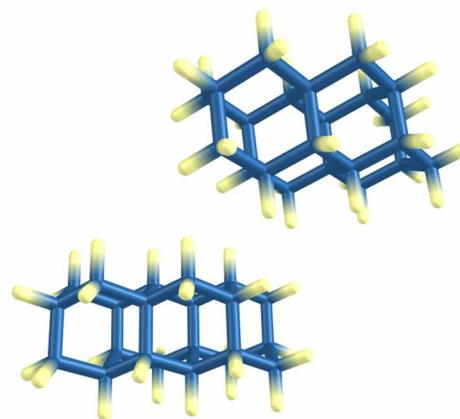
In addition to LD-bound dimers, we also computed LD-bound tetramers (consisting of four [121]tetramantane molecules, Figures S6 and S7). Due to the large size of such complexes, we did not perform structure optimization nor use any of the more time-consuming computational methods. Single-point energies were computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory using geometries obtained from experimental AFM imaging (Table S7). The resulting interaction energies (from electronic energies without ZPVEs) were sufficient for our purposes of comparing feasible tetramantane orientations on Au(111) and Cu(111) surfaces, as discussed in the text and Table 1 of the paper.



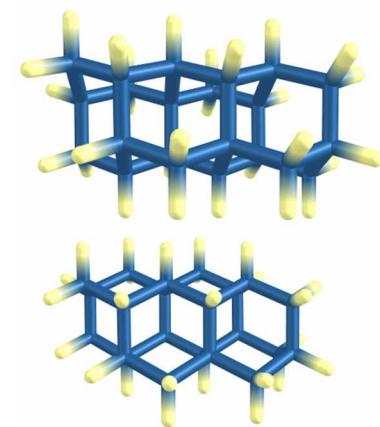
D1



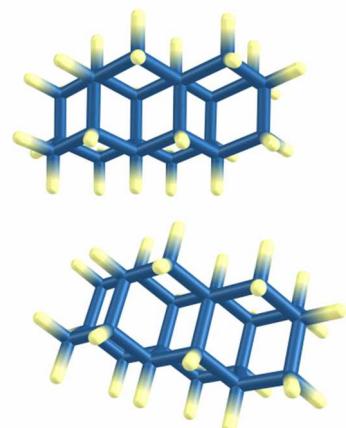
D2



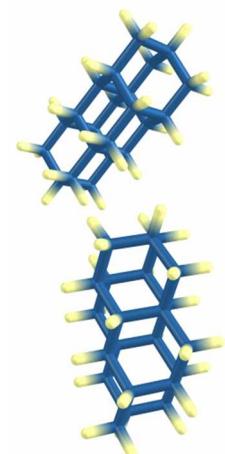
D3



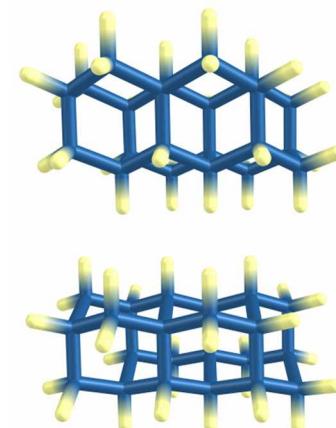
D4



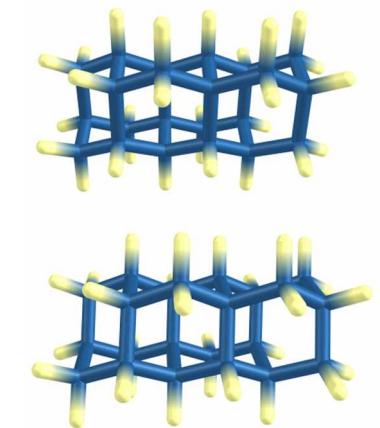
D5



D6



D7



D8

**Figure S9.** Optimized structures of [121]tetramantane LD-bound complexes (**D1-D8**) computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.

**Table S1.** Interaction energies,  $\Delta H(0\text{ K})$ , of [121]tetramantane LD-bound complexes (**D1–D8**) in kcal mol<sup>-1</sup>. Geometries for RI-MP2 and DLPNO-CCSD(T) single-point computations were optimized at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.<sup>a, b, c</sup>

Level of theory	<b>D1</b>	<b>D2</b>	<b>D3</b>	<b>D4</b>	<b>D5</b>	<b>D6</b>	<b>D7</b>	<b>D8</b>
B3LYP/6-31G(d,p)	0.0 (-0.3)	0.1(-0.3)	0.2 (-0.9)	0.1 (-0.4)	-0.2 (-0.2)	0.0 (-0.2)	-0.3 (-0.4)	-0.2 (-0.3)
B3LYP-D3(BJ)/6-31G(d,p)	-8.8 (-9.2)	-4.0 (-4.3)	-5.7 (-6.2)	-8.5 (-9.0)	-7.4 (-7.8)	-4.7 (-5.0)	-7.5 (-8.2)	-8.2 (-8.8)
M06-2X/6-31G(d,p)	-5.9 (-6.1)	-2.6 (-2.2)	-3.4 (-3.9)	-5.4 (-5.9)	-4.5 (-4.8)	-2.2 (-2.5)	-4.3 (-4.4)	-4.7 (-5.0)
RI-MP2/cc-pVDZ	-7.8 (-8.3)	-3.3 (-3.6)	-4.7 (-5.2)	-8.0 (-8.5)	-6.6 (-7.0)	-3.7 (-4.1)	-6.3 (-7.0)	-7.4 (-8.0)
RI-MP2/cc-pVTZ	-9.0 (-9.4)	-3.7 (-4.0)	-5.5 (-6.0)	-8.9 (-9.4)	-7.4 (-7.9)	-4.2 (-4.6)	-7.4 (-8.0)	-8.4 (-9.0)
RI-MP2/CBS	-9.9 (-10.3)	-4.0 (-4.3)	-6.1 (-6.6)	-9.7 (-10.2)	-8.1 (-8.5)	-4.6 (-5.0)	-8.1 (-8.8)	-9.2 (-9.7)
DLPNO-CCSD(T)/cc-pVDZ	-6.3 (-6.7)	-2.8 (-3.0)	-3.7 (-4.2)	-6.5 (-7.0)	-5.3 (-5.7)	-2.9 (-3.3)	-4.9 (-5.6)	-6.0 (-6.6)
DLPNO-CCSD(T)/CBS	-8.3 (-8.8)	-3.4 (-3.7)	-5.1 (-5.6)	-8.2 (-8.7)	-6.8 (-7.2)	-3.8 (-4.2)	-6.7 (-7.3)	-7.8 (-8.3)
LED – dispersion (CCSD) <sup>d</sup>	(-7.2)	(-2.8)	(-4.5)	(-6.8)	(-5.9)	(-3.8)	(-6.3)	(-6.8)

<sup>a</sup> Interaction energies are defined as a difference between the energy of the dimer and the energy of two [121]tetramantane molecules. <sup>b</sup> Values in parentheses correspond to computed  $\Delta E$  in kcal mol<sup>-1</sup>. <sup>c</sup> ZPVEs used to obtain  $\Delta H(0\text{ K})$  for RI-MP2 and DLPNO-CCSD(T) computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory. <sup>d</sup> Local Energy Decomposition analysis accounting for dispersion contributions implemented in ORCA 4.0.0 for the DLPNO-CCSD(T) method.

**Table S2.** Electronic energies of [121]tetramantane (**1**) and its LD-bound complexes (**D1–D8**) in hartree.<sup>a</sup>

Level of theory	<b>1</b>	<b>D1</b>	<b>D2</b>	<b>D3</b>	<b>D4</b>	<b>D5</b>	<b>D6</b>	<b>D7</b>	<b>D8</b>
B3LYP/6-31G(d,p)	-855.313202	-1710.626943	-1710.626857	-1710.627893	-1710.626966	-1710.626793	-1710.626767	-1710.626994	-1710.626942
B3LYP-D3(BJ)/6-31G(d,p)	-855.451196	-1710.917073	-1710.909230	-1710.912201	-1710.916759	-1710.914850	-1710.910362	-1710.915486	-1710.916415
M06-2X/6-31G(d,p)	-854.968081	-1709.945925	-1709.939673	-1709.942337	-1709.945609	-1709.943802	-1709.940113	-1709.943112	-1709.944125
RI-MP2/cc-pVDZ	-852.606501	-1705.226158	-1705.218717	-1705.221265	-1705.226489	-1705.224211	-1705.219475	-1705.224177	-1705.225754
RI-MP2/cc-pVTZ	-853.433192	-1706.881439	-1706.872705	-1706.875944	-1706.881375	-1706.878917	-1706.873655	-1706.879200	-1706.880687
RI-MP2/CBS	-853.843659	-1707.703749	-1707.694125	-1707.697804	-1707.703502	-1707.700887	-1707.695232	-1707.701311	-1707.702831
DLPNO-CCSD(T)/cc-pVDZ	-852.892982	-1705.796645	-1705.790795	-1705.792703	-1705.797136	-1705.795102	-1705.791176	-1705.794819	-1705.796474
DLPNO-CCSD(T)/CBS	-854.130140	-1708.274235	-1708.266203	-1708.269241	-1708.274149	-1708.271779	-1708.266933	-1708.271953	-1708.273550

<sup>a</sup> Values for RI-MP2/CBS and DLPNO-CCSD(T)/CBS obtained from Eq. 3 and 4.**Table S3.** Zero-point vibrational energies (ZPVEs) of [121]tetramantane (**1**) and its LD-bound complexes (**D1–D8**) in hartree computed at different levels of theory.

Level of theory	<b>1</b>	<b>D1</b>	<b>D2</b>	<b>D3</b>	<b>D4</b>	<b>D5</b>	<b>D6</b>	<b>D7</b>	<b>D8</b>
B3LYP/6-31G(d,p)	0.460249	0.920984	0.921106	0.922239	0.921231	0.920645	0.920814	0.920601	0.920722
B3LYP-D3(BJ)/6-31G(d,p)	0.461486	0.923665	0.923420	0.923756	0.923727	0.923704	0.923489	0.924042	0.923855
M06-2X/6-31G(d,p)	0.464412	0.929107	0.928232	0.929589	0.929602	0.929287	0.929259	0.928942	0.929351

**Table S4.** Geometries in Cartesian coordinates in Å computed at the B3LYP/6-31G(d,p) level of theory.

<b>1</b>			
6	-1.463864000	-1.310241000	1.255148000
6	-2.189572000	-0.766803000	0.0000000000
6	-1.463864000	-1.310241000	-1.255148000
6	-1.463864000	-2.849609000	1.256085000
6	0.712504000	-2.849993000	0.0000000000
6	-1.463864000	-2.849609000	-1.256085000
6	-0.737952000	-3.369302000	0.0000000000
6	-2.180665000	0.769998000	0.0000000000
6	0.013980000	0.771688000	1.251750000
6	-0.739875000	1.309419000	0.0000000000
6	0.013980000	0.771688000	-1.251750000
6	1.463864000	1.310241000	-1.255148000
6	2.189572000	0.766803000	0.0000000000
6	1.463864000	1.310241000	1.255148000
6	-0.013980000	-0.771688000	1.251750000
6	2.180665000	-0.769998000	0.0000000000
6	-0.013980000	-0.771688000	-1.251750000
6	0.739875000	-1.309419000	0.0000000000
6	-0.712504000	2.849993000	0.0000000000
6	1.463864000	2.849609000	-1.256085000
6	1.463864000	2.849609000	1.256085000
6	0.737952000	3.369302000	0.0000000000
1	-1.978454000	-0.942345000	2.154384000
1	-3.227874000	-1.127757000	0.0000000000
1	-1.978454000	-0.942345000	-2.154384000
1	-0.968226000	-3.224431000	2.161579000
1	-2.495464000	-3.225467000	1.279444000
1	1.249505000	-3.227276000	-0.881661000
1	1.249505000	-3.227276000	0.881661000
1	-0.968226000	-3.224431000	-2.161579000
1	-2.495464000	-3.225467000	-1.279444000
1	-0.736769000	-4.466773000	0.0000000000
1	-2.716400000	1.149712000	-0.881597000
1	-2.716400000	1.149712000	0.881597000
1	-0.503902000	1.135296000	2.152928000
1	-0.503902000	1.135296000	-2.152928000
1	1.978454000	0.942345000	-2.154384000
1	3.227874000	1.127757000	0.0000000000
1	1.978454000	0.942345000	2.154384000
1	0.503902000	-1.135296000	2.152928000
1	2.716400000	-1.149712000	0.881597000
1	2.716400000	-1.149712000	-0.881597000
1	0.503902000	-1.135296000	-2.152928000
1	-1.249505000	3.227276000	-0.881661000
1	-1.249505000	3.227276000	0.881661000
1	0.968226000	3.224431000	-2.161579000
1	2.495464000	3.225467000	-1.279444000

1	0.968226000	3.224431000	2.161579000
1	2.495464000	3.225467000	1.279444000
1	0.736769000	4.466773000	0.000000000

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**D1**

6	5.077418000	1.492985000	-1.056266000
6	3.580024000	1.708289000	-1.386399000
6	2.821779000	1.965853000	-0.061259000
6	5.654822000	2.723913000	-0.334606000
6	5.023583000	1.720573000	1.881097000
6	3.397390000	3.197224000	0.661219000
6	4.886729000	2.962603000	0.979970000
6	3.006383000	0.474066000	-2.100113000
6	4.632421000	-1.013913000	-0.865222000
6	3.133740000	-0.778714000	-1.216292000
6	2.383179000	-0.542354000	0.127136000
6	2.509433000	-1.798914000	1.020135000
6	4.006754000	-2.014144000	1.350276000
6	4.765037000	-2.271750000	0.025087000
6	5.203845000	0.236415000	-0.163201000
6	4.580101000	-0.779824000	2.064107000
6	2.954272000	0.708071000	0.828970000
6	4.452832000	0.472883000	1.180114000
6	2.562675000	-2.026293000	-1.917182000
6	1.932567000	-3.030133000	0.298546000
6	4.189455000	-3.502979000	-0.697654000
6	2.700017000	-3.268486000	-1.016356000
1	5.630025000	1.322697000	-1.991359000
1	3.477672000	2.588599000	-2.036712000
1	1.758055000	2.134281000	-0.283082000
1	6.722148000	2.570580000	-0.126433000
1	5.580807000	3.608073000	-0.981740000
1	4.495276000	1.882380000	2.831228000
1	6.079814000	1.550023000	2.132751000
1	2.837513000	3.384988000	1.587132000
1	3.281080000	4.090133000	0.032628000
1	5.298131000	3.839688000	1.495615000
1	1.949296000	0.641948000	-2.351239000
1	3.533369000	0.309844000	-3.050752000
1	5.187673000	-1.179103000	-1.801651000
1	1.318291000	-0.368461000	-0.094684000
1	1.956644000	-1.628733000	1.955083000
1	4.109109000	-2.894490000	2.000562000
1	5.828501000	-2.440250000	0.247382000
1	6.268150000	0.062222000	0.059068000
1	5.636933000	-0.947479000	2.315952000
1	4.052397000	-0.615591000	3.014350000
1	2.398943000	0.873268000	1.765340000
1	1.506150000	-1.855649000	-2.167878000
1	3.090161000	-2.187906000	-2.867783000

1	0.864767000	-2.877092000	0.090600000
1	2.006767000	-3.914262000	0.945657000
1	4.749319000	-3.690423000	-1.623643000
1	4.305686000	-4.396115000	-0.069362000
1	2.288727000	-4.145599000	-1.532013000
1	-5.364259000	1.648589000	-2.158790000
1	-5.716659000	-0.721021000	-1.291621000
1	-5.677792000	3.616842000	-0.656711000
1	-3.905433000	-0.263353000	-3.030230000
1	-4.423958000	3.943541000	-1.853250000
6	-4.639559000	1.837141000	-1.353782000
6	-4.667177000	3.329221000	-0.976071000
1	-6.077603000	-3.100864000	-0.432293000
1	-4.257077000	-2.631013000	-2.170418000
1	-6.022245000	1.236575000	0.206996000
6	-4.990934000	-0.537521000	-0.484048000
1	-2.960122000	2.024445000	-2.719449000
6	-3.203713000	-0.067455000	-2.207074000
6	-5.010121000	0.965134000	-0.131309000
6	-3.227969000	1.424258000	-1.838329000
1	-6.377479000	-1.133223000	1.073392000
6	-5.342102000	-2.901284000	0.358442000
6	-3.555589000	-2.437686000	-1.346675000
6	-5.367947000	-1.409328000	0.736652000
6	-3.575241000	-0.937917000	-0.994213000
1	-2.205298000	-0.349183000	-2.570833000
6	-3.656589000	3.596949000	0.156147000
1	-5.630902000	-3.513345000	1.223293000
6	-3.929877000	-3.291038000	-0.119853000
1	-2.556809000	-2.716579000	-1.711060000
1	-3.676013000	4.660369000	0.426659000
1	-3.910455000	-4.354460000	-0.390332000
1	-5.029110000	3.022683000	1.748002000
6	-4.011528000	1.243750000	1.030306000
1	-1.956425000	3.819015000	-1.188032000
6	-2.219061000	1.715175000	-0.700630000
6	-4.030660000	2.743527000	1.383025000
6	-2.244606000	3.207304000	-0.322741000
1	-5.381082000	0.655086000	2.607393000
6	-4.358823000	-1.118476000	1.874344000
6	-2.577063000	-0.659147000	0.167524000
6	-4.382906000	0.373237000	2.243228000
6	-2.595942000	0.843412000	0.520107000
1	-1.209018000	1.439244000	-1.037246000
6	-2.919803000	-3.023289000	1.012661000
1	-4.626757000	-1.718681000	2.755437000
6	-2.947236000	-1.531236000	1.390013000
1	-1.564606000	-0.930474000	-0.171065000
1	-3.328626000	2.936457000	2.206407000
1	-1.508233000	3.406905000	0.467252000

1	-3.163309000	-3.637363000	1.889941000
1	-3.680804000	0.568928000	3.066125000
1	-1.908912000	-3.311607000	0.694079000
1	-1.870032000	1.026847000	1.327482000
1	-2.222467000	-1.342550000	2.194871000

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**D2**

6	3.650305000	1.952552000	-0.791660000
6	3.117751000	1.723167000	0.643975000
6	4.329790000	1.611669000	1.600995000
6	4.505909000	3.230690000	-0.853514000
6	6.556321000	1.883873000	-0.309337000
6	5.185858000	2.889614000	1.540947000
6	5.705216000	3.099286000	0.105319000
6	2.270402000	0.442292000	0.702249000
6	3.655148000	-0.575372000	-1.149713000
6	3.102696000	-0.784527000	0.290816000
6	4.332630000	-0.915502000	1.236411000
6	5.173649000	-2.147046000	0.825796000
6	5.706251000	-1.917531000	-0.609780000
6	4.494237000	-1.805937000	-1.566842000
6	4.491353000	0.721022000	-1.202214000
6	6.553724000	-0.636746000	-0.667623000
6	5.168766000	0.380984000	1.183930000
6	5.721222000	0.590082000	-0.256592000
6	2.267732000	-2.078406000	0.343621000
6	4.318101000	-3.425219000	0.887486000
6	3.638205000	-3.083905000	-1.506965000
6	3.118805000	-3.293747000	-0.071374000
1	2.797908000	2.047386000	-1.479509000
1	2.502243000	2.584021000	0.941309000
1	3.964041000	1.462484000	2.627039000
1	4.858984000	3.396808000	-1.880059000
1	3.897740000	4.103579000	-0.581140000
1	7.426640000	1.787053000	0.354889000
1	6.949601000	2.026389000	-1.325734000
1	6.028897000	2.809997000	2.240226000
1	4.590305000	3.756081000	1.858077000
1	6.316315000	4.009815000	0.061435000
1	1.878214000	0.296779000	1.718957000
1	1.398838000	0.536295000	0.039027000
1	2.802051000	-0.474701000	-1.838599000
1	3.967071000	-1.059767000	2.265033000
1	6.025998000	-2.241987000	1.513740000
1	6.321701000	-2.778384000	-0.907311000
1	4.860031000	-1.656628000	-2.592851000
1	4.856906000	0.865237000	-2.230854000
1	6.947545000	-0.491353000	-1.683590000
1	7.424270000	-0.730896000	-0.003030000
1	6.021833000	0.280338000	1.872885000

1	1.874913000	-2.221048000	1.360170000
1	1.397109000	-1.981384000	-0.320288000
1	3.965003000	-3.591501000	1.913989000
1	4.926317000	-4.298045000	0.614973000
1	2.795189000	-3.004140000	-2.206249000
1	4.233725000	-3.950356000	-1.824210000
1	2.507780000	-4.204336000	-0.027594000
1	-5.593319000	1.965312000	2.118065000
1	-5.148381000	-0.538681000	2.270026000
1	-3.713436000	3.580199000	1.823810000
1	-7.264674000	0.305534000	1.121234000
1	-5.170176000	4.172405000	1.025194000
6	-5.056992000	2.004054000	1.159081000
6	-4.402995000	3.387359000	0.991127000
1	-4.709568000	-3.051095000	2.433690000
1	-6.826354000	-2.194711000	1.275369000
1	-3.275981000	1.066145000	1.969955000
6	-4.611052000	-0.505360000	1.309449000
1	-6.839586000	2.504747000	0.022266000
6	-6.702661000	0.347207000	0.177405000
6	-3.980599000	0.893464000	1.141588000
6	-6.057844000	1.732039000	0.009335000
1	-2.830734000	-1.437597000	2.124968000
6	-4.187963000	-2.998544000	1.468685000
6	-6.264319000	-2.155938000	0.331628000
6	-3.533956000	-1.615459000	1.298786000
6	-5.634427000	-0.759906000	0.163909000
1	-7.428109000	0.169204000	-0.629098000
6	-3.645010000	3.443705000	-0.349433000
1	-3.416584000	-3.780084000	1.481110000
6	-5.179022000	-3.249210000	0.315481000
1	-6.989973000	-2.331220000	-0.475050000
1	-3.177665000	4.429354000	-0.469902000
1	-5.646409000	-4.234825000	0.436068000
1	-1.833945000	2.525455000	0.440871000
6	-3.189609000	0.954431000	-0.198171000
1	-5.407375000	3.974620000	-1.515142000
6	-5.289985000	1.809969000	-1.332988000
6	-2.559714000	2.350424000	-0.365731000
6	-4.635977000	3.193083000	-1.502730000
1	-1.394942000	0.025039000	0.593439000
6	-2.766119000	-1.537664000	-0.043564000
6	-4.843352000	-0.699081000	-1.175786000
6	-2.121554000	-0.152753000	-0.212015000
6	-4.212970000	0.699819000	-1.343703000
1	-5.993173000	1.632244000	-2.159266000
6	-4.421082000	-3.193057000	-1.025107000
1	-1.983958000	-2.309993000	-0.056236000
6	-3.767011000	-1.809802000	-1.193226000
1	-5.547896000	-0.871831000	-2.004223000

1	-1.997836000	2.389310000	-1.309582000
1	-4.114316000	3.245756000	-2.467695000
1	-3.653903000	-3.978101000	-1.059079000
1	-1.561004000	-0.111350000	-1.156955000
1	-5.110671000	-3.385998000	-1.857749000
1	-3.675610000	0.733182000	-2.304266000
1	-3.230750000	-1.771190000	-2.152262000

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### D3

6	-2.959673000	-1.687702000	-1.371041000
6	-2.072673000	-0.757481000	-0.508005000
6	-2.350556000	-1.065678000	0.983764000
6	-2.657673000	-3.164661000	-1.059812000
6	-4.420350000	-3.147127000	0.731113000
6	-2.048049000	-2.542182000	1.296664000
6	-2.940373000	-3.449960000	0.428104000
6	-2.382643000	0.715601000	-0.817292000
6	-4.771377000	0.111340000	-1.373569000
6	-3.857229000	1.038892000	-0.520367000
6	-4.163816000	0.731437000	0.974812000
6	-5.646179000	1.053452000	1.277039000
6	-6.533478000	0.123362000	0.413985000
6	-6.255303000	0.431699000	-1.077759000
6	-4.442044000	-1.365504000	-1.068700000
6	-6.223326000	-1.349821000	0.722921000
6	-3.834433000	-0.745338000	1.279665000
6	-4.748603000	-1.672897000	0.426500000
6	-4.185377000	2.513142000	-0.824894000
6	-5.948104000	2.530472000	0.966045000
6	-6.557739000	1.908330000	-1.390448000
6	-5.665285000	2.815963000	-0.521819000
1	-2.761295000	-1.488123000	-2.433856000
1	-1.015009000	-0.963493000	-0.727030000
1	-1.715146000	-0.420531000	1.607392000
1	-3.274619000	-3.815642000	-1.693554000
1	-1.609447000	-3.391662000	-1.295834000
1	-4.642462000	-3.362824000	1.785692000
1	-5.070490000	-3.799980000	0.131849000
1	-2.225507000	-2.744264000	2.361410000
1	-0.988282000	-2.757432000	1.104775000
1	-2.726215000	-4.503025000	0.650800000
1	-1.733632000	1.370732000	-0.218760000
1	-2.162998000	0.933394000	-1.872128000
1	-4.569281000	0.306882000	-2.438177000
1	-3.524319000	1.373394000	1.600461000
1	-5.844647000	0.853784000	2.339821000
1	-7.590786000	0.329446000	0.633010000
1	-6.890340000	-0.213439000	-1.701701000
1	-5.081571000	-2.007445000	-1.694329000
1	-6.871779000	-2.004846000	0.123881000

1	-6.443539000	-1.567896000	1.777593000
1	-4.036451000	-0.940900000	2.344287000
1	-3.535140000	3.165869000	-0.225609000
1	-3.963225000	2.728922000	-1.879446000
1	-5.331083000	3.181308000	1.599870000
1	-6.996292000	2.757555000	1.202107000
1	-6.380177000	2.110558000	-2.455164000
1	-7.617271000	2.123793000	-1.198140000
1	-5.879469000	3.869049000	-0.744399000
1	7.205197000	-0.181607000	0.925742000
1	5.667838000	1.752509000	1.548415000
1	6.655466000	-2.519007000	1.605937000
1	6.908423000	1.785934000	-0.681130000
1	7.511074000	-2.507019000	0.063726000
6	6.361502000	-0.700771000	0.448838000
6	6.569457000	-2.222503000	0.552024000
1	4.136002000	3.699522000	2.177634000
1	5.378420000	3.720714000	-0.061332000
1	5.114803000	-0.574258000	2.220501000
6	4.819807000	1.237048000	1.071276000
1	7.205555000	-0.535261000	-1.546332000
6	6.057274000	1.255541000	-1.131302000
6	5.051674000	-0.286457000	1.159513000
6	6.272032000	-0.263069000	-1.033678000
1	3.578981000	1.360357000	2.845692000
6	3.306355000	3.174157000	1.685979000
6	4.525843000	3.192576000	-0.511027000
6	3.513365000	1.652242000	1.787723000
6	4.756801000	1.671743000	-0.422491000
1	6.016886000	1.563133000	-2.185898000
6	5.385907000	-2.954208000	-0.110250000
1	2.388387000	3.464737000	2.214108000
6	3.219828000	3.588261000	0.204102000
1	4.486877000	3.497627000	-1.566227000
1	5.532788000	-4.039292000	-0.036549000
1	3.072969000	4.673349000	0.130360000
1	4.118960000	-2.863563000	1.660167000
6	3.849022000	-1.037725000	0.516389000
1	6.217275000	-2.830678000	-2.120301000
6	5.092408000	-1.018131000	-1.693753000
6	4.079975000	-2.558535000	0.604961000
6	5.299358000	-2.540054000	-1.592120000
1	2.589266000	-0.928906000	2.280098000
6	2.333859000	0.897108000	1.127586000
6	3.554115000	0.920484000	-1.065594000
6	2.548898000	-0.621371000	1.225508000
6	3.785971000	-0.602983000	-0.977353000
1	5.026821000	-0.726183000	-2.751703000
6	2.036416000	2.856480000	-0.458305000
1	1.400110000	1.169000000	1.640166000

6	2.244415000	1.334830000	-0.354876000
1	3.490932000	1.208269000	-2.126588000
1	3.227332000	-3.086663000	0.155348000
1	4.469657000	-3.065371000	-2.083734000
1	1.094519000	3.140975000	0.029632000
1	1.697461000	-1.151940000	0.775428000
1	1.950421000	3.152805000	-1.512233000
1	2.937821000	-1.118362000	-1.454443000
1	1.400225000	0.815989000	-0.831643000

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**D4**

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6	-5.316261000	-2.703449000	-0.976519000
6	-4.879114000	-2.087800000	1.420066000
6	-3.079629000	-3.191812000	0.057062000
6	-4.596814000	-3.127427000	0.318992000
6	-2.775244000	0.017646000	-2.131409000
6	-4.575936000	1.130782000	-0.752450000
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6	-4.854548000	2.188191000	0.341325000
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6	-2.827782000	3.504671000	-0.366639000
1	-5.324077000	-1.019727000	-2.345983000
1	-3.076927000	-2.099562000	-2.484068000
1	-1.488632000	-1.861237000	-0.573584000
1	-6.401513000	-2.667841000	-0.812183000
1	-5.138556000	-3.444056000	-1.767679000
1	-4.386957000	-2.385284000	2.356716000
1	-5.956946000	-2.042870000	1.630590000
1	-2.550377000	-3.507752000	0.966044000
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1	-3.265941000	0.319094000	-3.067756000
1	-5.095205000	1.428010000	-1.676857000
1	-1.262940000	0.588247000	0.099015000
1	-2.103245000	1.396895000	2.298296000
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1	-5.937943000	2.236625000	0.522128000

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1	-2.330020000	-1.050861000	1.627580000
1	-1.467300000	2.419249000	-1.677435000
1	-3.036380000	2.763127000	-2.405019000
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1	-4.871932000	3.887062000	-1.016872000
1	-4.564883000	4.319893000	0.665072000
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1	5.935700000	0.166608000	-1.029299000
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6	4.532392000	-2.216162000	-0.783084000
6	4.283184000	-3.579386000	-0.113010000
1	6.479391000	2.629504000	-0.616656000
1	4.934051000	1.966871000	-2.547888000
1	5.699637000	-1.422686000	0.864953000
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1	3.101106000	-2.535251000	-2.386171000
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6	4.809005000	-1.133059000	0.285831000
6	3.297246000	-1.782058000	-1.609941000
1	6.235122000	1.032824000	1.285611000
6	5.598862000	2.689593000	0.036853000
6	4.081934000	2.036943000	-1.857248000
6	5.347435000	1.326910000	0.707445000
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6	1.826941000	-3.067357000	0.011546000
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6	2.616590000	0.755840000	-0.237276000
6	3.876703000	0.040506000	2.319790000
6	2.361322000	-0.622314000	0.409678000
1	1.189864000	-1.410693000	-1.236245000

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6	2.893236000	1.839185000	0.831570000
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1	2.491270000	-2.344437000	2.596174000
1	0.946604000	-3.008355000	0.666138000
1	3.319120000	3.970430000	0.926360000
1	3.023934000	0.108011000	3.010146000
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1	2.021932000	1.911991000	1.498352000

### D5

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6	-3.262865000	2.415311000	-1.293179000
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6	-4.511427000	3.139614000	-0.754563000
6	-5.732644000	-0.551943000	1.269625000
6	-4.487293000	-1.251209000	-0.814188000
6	-4.492258000	-1.293652000	0.742161000
6	-3.206735000	-0.557887000	1.222368000
6	-1.957096000	-1.299455000	0.692857000
6	-1.977841000	-1.247910000	-0.854334000
6	-3.240781000	-1.994592000	-1.349090000
6	-4.518267000	0.215594000	-1.294062000
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6	-1.949472000	-2.757571000	1.185879000
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6	-3.213169000	-3.482018000	0.682858000
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1	-2.351983000	2.930709000	-0.957426000
1	-3.253989000	2.442696000	-2.391910000
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1	-5.391708000	-1.762317000	-1.179297000
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1	4.010736000	-0.307159000	3.073520000
1	4.511274000	3.923323000	1.977110000
6	4.723165000	1.827951000	1.431954000
6	4.744950000	3.327477000	1.084716000
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1	4.354610000	-2.656380000	2.161211000
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6	5.066469000	-0.527980000	0.509636000
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6	3.299204000	-0.095282000	2.262827000
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6	3.317739000	1.403707000	1.924464000
1	6.435115000	-1.090234000	-1.075824000
6	5.409616000	-2.873696000	-0.385283000
6	3.643112000	-2.446998000	1.350067000
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6	4.081450000	2.789373000	-1.278404000
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6	4.407213000	-1.061403000	-1.852689000
6	2.645265000	-0.639141000	-0.115847000
6	4.425589000	0.437604000	-2.191156000

6	2.658628000	0.870284000	-0.437792000
1	1.289682000	1.432506000	1.147475000
6	2.979750000	-2.984957000	-1.013022000
1	4.665397000	-1.643130000	-2.748957000
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1	3.212971000	-3.581042000	-1.905378000
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### D6

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6	3.181687000	2.977234000	-1.240221000
6	2.520092000	2.760630000	0.134735000
6	6.729599000	1.635403000	-0.343837000
6	5.693424000	-0.086030000	1.187561000
6	6.385686000	0.143981000	-0.188065000
6	5.363404000	-0.268790000	-1.287530000
6	5.013470000	-1.767553000	-1.133736000
6	4.332323000	-1.970927000	0.241878000
6	5.344368000	-1.584266000	1.348082000
6	4.434084000	0.800482000	1.290286000
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6	3.411824000	0.387647000	0.190716000
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6	6.284804000	-2.628747000	-1.240695000
6	6.615862000	-2.445408000	1.242926000
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1	3.770902000	4.224221000	1.154344000
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1	7.220660000	1.801170000	-1.313267000
1	7.453026000	1.929535000	0.429822000
1	6.396491000	0.203971000	1.983862000

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1	4.877045000	-1.737971000	2.331331000
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6	-6.395776000	2.261087000	0.063645000
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1	-3.556789000	-3.482969000	0.775114000
6	-4.503795000	-1.715996000	-0.058921000
1	-0.804120000	-0.746020000	-1.128888000
6	-2.883571000	-0.107536000	-1.162840000
6	-3.401867000	-2.792894000	-0.066208000
6	-1.802103000	-1.202710000	-1.173041000
1	-6.058392000	-3.032799000	0.688502000
6	-6.992283000	-1.254730000	-0.144299000

6	-5.396191000	0.337905000	-1.246602000
6	-5.906042000	-2.341820000	-0.152770000
6	-4.291841000	-0.740571000	-1.253883000
1	-2.737284000	0.561230000	-2.023178000
6	-7.885886000	0.800343000	-1.336240000
1	-7.983182000	-1.725808000	-0.212092000
6	-6.804147000	-0.294748000	-1.344468000
1	-5.244286000	1.006021000	-2.108622000
1	-3.479726000	-3.392217000	-0.984252000
1	-1.851110000	-1.769993000	-2.112144000
1	-8.881497000	0.345860000	-1.426913000
1	-5.981167000	-2.941981000	-1.070696000
1	-7.757652000	1.461127000	-2.203980000
1	-4.364896000	-1.315764000	-2.190025000
1	-6.871826000	-0.870792000	-2.278492000

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**D7**

6	-5.059769000	2.139574000	-0.210559000
6	-4.682087000	1.857004000	1.264167000
6	-3.137838000	1.830689000	1.374501000
6	-4.462638000	3.480272000	-0.674752000
6	-2.384844000	2.290297000	-1.436774000
6	-2.539135000	3.170982000	0.911243000
6	-2.926783000	3.432911000	-0.557019000
6	-5.274251000	0.514394000	1.720753000
6	-5.107904000	-0.377323000	-0.637127000
6	-4.745002000	-0.641094000	0.853839000
6	-3.191090000	-0.685430000	0.943686000
6	-2.654534000	-1.844980000	0.072103000
6	-3.031913000	-1.562338000	-1.402629000
6	-4.576183000	-1.535982000	-1.512934000
6	-4.522934000	0.980026000	-1.082082000
6	-2.439786000	-0.219759000	-1.859083000
6	-2.606403000	0.671963000	0.498717000
6	-2.968929000	0.935704000	-0.992247000
6	-5.329271000	-1.995711000	1.298384000
6	-3.251479000	-3.185734000	0.536274000
6	-5.174827000	-2.876408000	-1.049838000
6	-4.787276000	-3.138303000	0.418507000
1	-6.155022000	2.174789000	-0.299840000
1	-5.074471000	2.665286000	1.897468000
1	-2.856169000	1.644642000	2.420826000
1	-4.756239000	3.682451000	-1.713475000
1	-4.863443000	4.301236000	-0.065349000
1	-1.287686000	2.254869000	-1.377272000
1	-2.637543000	2.471637000	-2.490955000
1	-1.446054000	3.149718000	1.015654000
1	-2.903763000	3.986388000	1.550128000
1	-2.499920000	4.388064000	-0.888440000
1	-5.021394000	0.330279000	2.774591000

1	-6.371444000	0.547040000	1.661369000
1	-6.204652000	-0.336594000	-0.726519000
1	-2.908036000	-0.866385000	1.992294000
1	-1.558896000	-1.880438000	0.161381000
1	-2.639546000	-2.370602000	-2.035951000
1	-4.857761000	-1.349924000	-2.559309000
1	-4.805858000	1.160987000	-2.130757000
1	-2.692131000	-0.035612000	-2.913049000
1	-1.342382000	-0.252461000	-1.799482000
1	-1.509296000	0.631262000	0.588239000
1	-5.076080000	-2.177126000	2.352420000
1	-6.426205000	-1.960219000	1.239090000
1	-2.957821000	-3.387858000	1.574966000
1	-2.850606000	-4.006617000	-0.073173000
1	-6.267821000	-2.855371000	-1.154534000
1	-4.809808000	-3.691706000	-1.688632000
1	-5.214136000	-4.093501000	0.749857000
1	4.857840000	1.350080000	2.559182000
1	4.805896000	-1.160859000	2.130802000
1	6.267888000	2.855411000	1.154272000
1	2.692199000	0.035824000	2.913065000
1	4.809899000	3.691803000	1.688347000
6	4.576239000	1.536070000	1.512801000
6	5.174892000	2.876456000	1.049600000
1	4.756235000	-3.682353000	1.713691000
1	2.637592000	-2.471455000	2.491146000
1	6.204674000	0.336608000	0.726428000
6	4.522948000	-0.979966000	1.082122000
1	2.639627000	2.370753000	2.035807000
6	2.439834000	0.219901000	1.859092000
6	5.107925000	0.377345000	0.637060000
6	3.031967000	1.562441000	1.402530000
1	6.155001000	-2.174804000	0.299920000
6	4.462609000	-3.480239000	0.674963000
6	2.384854000	-2.290185000	1.436963000
6	5.059745000	-2.139580000	0.210664000
6	2.968941000	-0.935629000	0.992324000
1	1.342430000	0.252614000	1.799512000
6	4.787310000	3.138257000	-0.418754000
1	4.863387000	-4.301249000	0.065604000
6	2.926751000	-3.432865000	0.557267000
1	1.287695000	-2.254749000	1.377505000
1	5.214175000	4.093426000	-0.750180000
1	2.499884000	-4.387989000	0.888764000
1	6.426202000	1.960093000	-1.239296000
6	4.744990000	0.641019000	-0.853915000
1	2.850663000	4.006632000	0.072912000
6	2.654557000	1.844987000	-0.072212000
6	5.329268000	1.995597000	-1.298567000
6	3.251511000	3.185701000	-0.536488000

1	6.371395000	-0.547193000	-1.661405000
6	4.682030000	-1.857106000	-1.264071000
6	2.606381000	-0.671985000	-0.498649000
6	5.274201000	-0.514535000	-1.720764000
6	3.191076000	0.685370000	-0.943727000
1	1.558918000	1.880457000	-0.161472000
6	2.539067000	-3.171030000	-0.911002000
1	5.074387000	-2.665436000	-1.897326000
6	3.137778000	-1.830777000	-1.374368000
1	1.509272000	-0.631276000	-0.588144000
1	5.076054000	2.176944000	-2.352609000
1	2.957832000	3.387758000	-1.575187000
1	2.903666000	-3.986485000	-1.549841000
1	5.021320000	-0.330488000	-2.774608000
1	1.445984000	-3.149756000	-1.015385000
1	2.908000000	0.866255000	-1.992341000
1	2.856085000	-1.644799000	-2.420699000

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6	5.412219000	-1.536174000	-0.823543000
6	5.293691000	-1.609788000	0.718479000
6	3.810782000	-1.869347000	1.080753000
6	4.920626000	-2.845270000	-1.467029000
6	2.595242000	-1.904422000	-1.603488000
6	3.317799000	-3.178419000	0.438566000
6	3.444538000	-3.084494000	-1.094354000
6	5.778633000	-0.298258000	1.355904000
6	5.040224000	0.986332000	-0.690631000
6	4.941842000	0.893854000	0.860504000
6	3.443218000	0.653842000	1.208622000
6	2.597373000	1.849253000	0.711136000
6	2.715735000	1.923121000	-0.830794000
6	4.198645000	2.182763000	-1.193254000
6	4.566655000	-0.340545000	-1.321195000
6	2.231505000	0.611838000	-1.468847000
6	2.969630000	-0.672858000	0.577911000
6	3.067994000	-0.580547000	-0.973248000
6	5.415014000	2.217901000	1.490386000
6	3.088927000	3.158259000	1.354798000
6	4.691336000	3.492045000	-0.551005000
6	4.564876000	3.397717000	0.981884000
1	6.464004000	-1.366050000	-1.094764000
1	5.905726000	-2.445114000	1.087204000
1	3.715316000	-1.937679000	2.173888000
1	5.031235000	-2.791807000	-2.558317000
1	5.537941000	-3.686885000	-1.125606000
1	1.535517000	-2.068983000	-1.361996000
1	2.661637000	-1.834959000	-2.698361000
1	2.272990000	-3.364689000	0.721144000
1	3.905043000	-4.026471000	0.815281000

1	3.092989000	-4.017267000	-1.553365000
1	5.712778000	-0.365006000	2.451161000
1	6.837817000	-0.131009000	1.113865000
1	6.094120000	1.151655000	-0.963544000
1	3.347665000	0.579589000	2.303077000
1	1.545574000	1.678761000	0.982400000
1	2.103647000	2.758462000	-1.199409000
1	4.293830000	2.251332000	-2.286407000
1	4.662353000	-0.266503000	-2.415646000
1	2.297980000	0.678687000	-2.564015000
1	1.171866000	0.443921000	-1.227775000
1	1.915391000	-0.837866000	0.850932000
1	5.349256000	2.148258000	2.585298000
1	6.474322000	2.382503000	1.247926000
1	2.978558000	3.104490000	2.446103000
1	2.471290000	3.999791000	1.013729000
1	5.736011000	3.678685000	-0.833576000
1	4.103614000	4.339842000	-0.927561000
1	4.916308000	4.330544000	1.440932000
1	-6.131697000	0.195109000	-2.133541000
1	-5.316158000	-1.958632000	-1.043994000
1	-7.305389000	1.940128000	-0.789875000
1	-3.962219000	-0.900387000	-2.930650000
1	-6.372118000	2.682057000	-2.089557000
6	-5.566014000	0.783773000	-1.397202000
6	-6.283637000	2.122746000	-1.148646000
1	-4.503935000	-4.126106000	0.039031000
1	-3.146429000	-3.052596000	-1.849277000
1	-6.477651000	-0.219819000	0.297095000
6	-4.747117000	-1.373743000	-0.304739000
1	-4.194921000	1.583167000	-2.881062000
6	-3.419906000	-0.313988000	-2.175441000
6	-5.462631000	-0.024261000	-0.082420000
6	-4.134569000	1.025198000	-1.935915000
1	-5.664789000	-2.374920000	1.385911000
6	-3.934086000	-3.524488000	0.759634000
6	-2.603701000	-2.468729000	-1.092665000
6	-4.649784000	-2.184643000	1.008619000
6	-3.318435000	-1.122065000	-0.870315000
1	-2.412580000	-0.136704000	-2.578184000
6	-5.497045000	2.948553000	-0.112358000
1	-3.886663000	-4.104255000	1.691066000
6	-2.512723000	-3.261980000	0.224880000
1	-1.597140000	-2.288444000	-1.495941000
1	-6.008181000	3.903147000	0.066166000
1	-2.001536000	-4.216541000	0.046481000
1	-6.411701000	1.975647000	1.609289000
6	-4.691045000	0.808791000	0.982823000
1	-4.123470000	3.790614000	-1.578965000
6	-3.359862000	1.871390000	-0.896195000

6	-5.405484000	2.155589000	1.205341000
6	-4.075839000	3.211133000	-0.647360000
1	-5.596904000	-0.176442000	2.690890000
6	-3.875172000	-1.338577000	2.048446000
6	-2.547107000	-0.289040000	0.195122000
6	-4.589592000	0.000810000	2.288012000
6	-3.262370000	1.060444000	0.417206000
1	-2.344835000	2.061670000	-1.273458000
6	-1.726790000	-2.436449000	1.261876000
1	-3.814821000	-1.896535000	2.993608000
6	-2.443676000	-1.097033000	1.509838000
1	-1.531590000	-0.094351000	-0.185001000
1	-4.861934000	2.739500000	1.961355000
1	-3.505956000	3.813092000	0.072937000
1	-1.638972000	-2.995745000	2.202838000
1	-4.047162000	0.587037000	3.043282000
1	-0.704337000	-2.254207000	0.903778000
1	-2.693240000	1.645361000	1.156388000
1	-1.877963000	-0.508465000	2.246208000

**Table S5.** Geometries in Cartesian coordinates in Å computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.

<b>1</b>			
6	-1.459144000	-1.304892000	1.252854000
6	-2.183506000	-0.764961000	0.000000000
6	-1.459144000	-1.304892000	-1.252854000
6	-1.459144000	-2.840782000	1.254334000
6	0.712240000	-2.839872000	0.000000000
6	-1.459144000	-2.840782000	-1.254334000
6	-0.734729000	-3.359348000	0.000000000
6	-2.174761000	0.767973000	0.000000000
6	0.013142000	0.769118000	1.248937000
6	-0.737184000	1.303767000	0.000000000
6	0.013142000	0.769118000	-1.248937000
6	1.459144000	1.304892000	-1.252854000
6	2.183506000	0.764961000	0.000000000
6	1.459144000	1.304892000	1.252854000
6	-0.013142000	-0.769118000	1.248937000
6	2.174761000	-0.767973000	0.000000000
6	-0.013142000	-0.769118000	-1.248937000
6	0.737184000	-1.303767000	0.000000000
6	-0.712240000	2.839872000	0.000000000
6	1.459144000	2.840782000	-1.254334000
6	1.459144000	2.840782000	1.254334000
6	0.734729000	3.359348000	0.000000000
1	-1.972854000	-0.934001000	2.150347000
1	-3.219854000	-1.128971000	0.000000000
1	-1.972854000	-0.934001000	-2.150347000

1	-0.961300000	-3.214247000	2.158372000
1	-2.490292000	-3.215958000	1.276647000
1	1.249075000	-3.214034000	-0.882193000
1	1.249075000	-3.214034000	0.882193000
1	-0.961300000	-3.214247000	-2.158372000
1	-2.490292000	-3.215958000	-1.276647000
1	-0.733329000	-4.456093000	0.000000000
1	-2.707453000	1.148351000	-0.882202000
1	-2.707453000	1.148351000	0.882202000
1	-0.506545000	1.133711000	2.147518000
1	-0.506545000	1.133711000	-2.147518000
1	1.972854000	0.934001000	-2.150347000
1	3.219854000	1.128971000	0.000000000
1	1.972854000	0.934001000	2.150347000
1	0.506545000	-1.133711000	2.147518000
1	2.707453000	-1.148351000	0.882202000
1	2.707453000	-1.148351000	-0.882202000
1	0.506545000	-1.133711000	-2.147518000
1	-1.249075000	3.214034000	-0.882193000
1	-1.249075000	3.214034000	0.882193000
1	0.961300000	3.214247000	-2.158372000
1	2.490292000	3.215958000	-1.276647000
1	0.961300000	3.214247000	2.158372000
1	2.490292000	3.215958000	1.276647000
1	0.733329000	4.456093000	0.000000000

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6	4.878683000	-0.933608000	0.920161000
6	3.583253000	-1.129746000	1.738293000
6	2.505744000	-1.730343000	0.809427000
6	5.356766000	-2.273089000	0.340490000
6	3.990091000	-1.865819000	-1.722587000
6	2.981147000	-3.070732000	0.230458000
6	4.270573000	-2.855737000	-0.580351000
6	3.104805000	0.210264000	2.308463000
6	4.111941000	1.420905000	0.340976000
6	2.823888000	1.211924000	1.181185000
6	1.746469000	0.627152000	0.230279000
6	1.458945000	1.630113000	-0.904327000
6	2.753328000	1.825847000	-1.723198000
6	3.831792000	2.426129000	-0.794243000
6	4.591098000	0.069105000	-0.215266000
6	3.228047000	0.484597000	-2.293548000
6	2.225536000	-0.724569000	-0.325083000
6	3.512606000	-0.515984000	-1.166102000
6	2.343522000	2.560827000	1.737520000
6	0.980713000	2.968743000	-0.324089000
6	3.356935000	3.766760000	-0.214757000
6	2.066919000	3.551851000	0.595318000
1	5.655428000	-0.515434000	1.574972000

1	3.780361000	-1.831820000	2.559721000
1	1.584223000	-1.883443000	1.385334000
1	6.288293000	-2.126690000	-0.221154000
1	5.578507000	-2.976029000	1.153650000
1	3.225253000	-2.273476000	-2.397454000
1	4.896920000	-1.713487000	-2.323305000
1	2.201011000	-3.500853000	-0.410220000
1	3.159655000	-3.787109000	1.042478000
1	4.610984000	-3.812051000	-0.995555000
1	2.192117000	0.062801000	2.902000000
1	3.862902000	0.624660000	2.986868000
1	4.892260000	1.831511000	0.998945000
1	0.826364000	0.468178000	0.808944000
1	0.682655000	1.212396000	-1.559509000
1	2.555709000	2.527995000	-2.544455000
1	4.755034000	2.577944000	-1.370035000
1	5.512916000	0.229194000	-0.794146000
1	4.137045000	0.629475000	-2.893045000
1	2.465092000	0.070035000	-2.966609000
1	1.446205000	-1.134412000	-0.984173000
1	1.433063000	2.406397000	2.332524000
1	3.103979000	2.967982000	2.417414000
1	0.053336000	2.821083000	0.240814000
1	0.752892000	3.671012000	-1.136191000
1	4.137946000	4.195033000	0.426459000
1	3.177473000	4.483796000	-1.026028000
1	1.726053000	4.508113000	1.010296000
1	-4.755033000	-2.577951000	1.370025000
1	-5.512915000	-0.229198000	0.794149000
1	-4.137947000	-4.195031000	-0.426478000
1	-4.137042000	-0.629490000	2.893044000
1	-3.177473000	-4.483802000	1.026006000
6	-3.831791000	-2.426133000	0.794233000
6	-3.356935000	-3.766761000	0.214740000
1	-6.288293000	2.126689000	0.221170000
1	-4.896918000	1.713474000	2.323318000
1	-4.892261000	-1.831505000	-0.998952000
6	-4.591098000	-0.069106000	0.215268000
1	-2.555707000	-2.528008000	2.544443000
6	-3.228045000	-0.484609000	2.293548000
6	-4.111941000	-1.420903000	-0.340981000
6	-2.753327000	-1.825856000	1.723190000
1	-5.655430000	0.515442000	-1.574965000
6	-5.356767000	2.273090000	-0.340475000
6	-3.990089000	1.865810000	1.722599000
6	-4.878684000	0.933613000	-0.920153000
6	-3.512605000	0.515978000	1.166106000
1	-2.465090000	-0.070050000	2.966610000
6	-2.066920000	-3.551847000	-0.595335000
1	-5.578508000	2.976036000	-1.153630000

6	-4.270572000	2.855734000	0.580368000
1	-3.225251000	2.273463000	2.397468000
1	-1.726054000	-4.508108000	-1.010319000
1	-4.610983000	3.812046000	0.995578000
1	-3.103981000	-2.967969000	-2.417428000
6	-2.823889000	-1.211918000	-1.181190000
1	-0.752892000	-3.671018000	1.136172000
6	-1.458944000	-1.630117000	0.904319000
6	-2.343524000	-2.560818000	-1.737532000
6	-0.980713000	-2.968745000	0.324074000
1	-3.862905000	-0.624645000	-2.986869000
6	-3.583254000	1.129755000	-1.738285000
6	-2.225536000	0.724568000	0.325087000
6	-3.104808000	-0.210252000	-2.308463000
6	-1.746469000	-0.627151000	-0.230282000
1	-0.682654000	-1.212404000	1.559502000
6	-2.981147000	3.070734000	-0.230440000
1	-3.780363000	1.831834000	-2.559709000
6	-2.505744000	1.730347000	-0.809417000
1	-1.446205000	1.134407000	0.984179000
1	-1.433065000	-2.406385000	-2.332536000
1	-0.053336000	-2.821081000	-0.240828000
1	-3.159656000	3.787115000	-1.042457000
1	-2.192120000	-0.062786000	-2.902000000
1	-2.201010000	3.500850000	0.410239000
1	-0.826364000	-0.468174000	-0.808947000
1	-1.584225000	1.883451000	-1.385324000

## D2

6	-3.115456000	-1.838969000	-0.749827000
6	-2.623938000	-1.596023000	0.693925000
6	-3.855589000	-1.485379000	1.618346000
6	-3.956839000	-3.121589000	-0.823067000
6	-6.025528000	-1.788605000	-0.340704000
6	-4.698130000	-2.767512000	1.547977000
6	-5.178280000	-2.992184000	0.103621000
6	-1.791909000	-0.311807000	0.757489000
6	-3.132011000	0.677082000	-1.126641000
6	-2.621864000	0.901036000	0.321681000
6	-3.869488000	1.030098000	1.234067000
6	-4.707969000	2.247322000	0.794330000
6	-5.200416000	2.004405000	-0.649435000
6	-3.968055000	1.893020000	-1.573950000
6	-3.954253000	-0.621659000	-1.189795000
6	-6.033902000	0.719448000	-0.717669000
6	-4.691888000	-0.268820000	1.171162000
6	-5.202754000	-0.492736000	-0.277113000
6	-1.796772000	2.195885000	0.383512000
6	-3.865238000	3.529494000	0.867075000
6	-3.124709000	3.174823000	-1.503691000

6	-2.643993000	3.399668000	-0.059508000
1	-2.243666000	-1.928904000	-1.412603000
1	-2.009443000	-2.449574000	1.011617000
1	-3.514824000	-1.322236000	2.649984000
1	-4.284426000	-3.296578000	-1.855869000
1	-3.348788000	-3.986105000	-0.527396000
1	-6.911145000	-1.691015000	0.301633000
1	-6.390298000	-1.939850000	-1.365671000
1	-5.559733000	-2.687468000	2.223140000
1	-4.103390000	-3.625926000	1.885581000
1	-5.780815000	-3.907133000	0.051785000
1	-1.415648000	-0.153588000	1.777732000
1	-0.916668000	-0.404367000	0.106735000
1	-2.258861000	0.578115000	-1.788867000
1	-3.527486000	1.184821000	2.268279000
1	-5.578512000	2.338536000	1.458261000
1	-5.812052000	2.859187000	-0.968504000
1	-4.308760000	1.730352000	-2.605677000
1	-4.295958000	-0.776559000	-2.224065000
1	-6.399074000	0.560609000	-1.741484000
1	-6.919551000	0.809647000	-0.074074000
1	-5.564090000	-0.170128000	1.834461000
1	-1.428357000	2.346407000	1.407359000
1	-0.913184000	2.098127000	-0.260333000
1	-3.537407000	3.703745000	1.899913000
1	-4.472504000	4.394753000	0.571896000
1	-2.263118000	3.093324000	-2.178759000
1	-3.718478000	4.033644000	-1.841917000
1	-2.041167000	4.314490000	-0.008247000
1	4.846118000	-2.386293000	1.915534000
1	5.064867000	0.128658000	2.149079000
1	2.599821000	-3.470291000	1.856092000
1	6.732138000	-1.155096000	0.728797000
1	3.751503000	-4.370642000	0.866866000
6	4.200007000	-2.252797000	1.037093000
6	3.207119000	-3.420741000	0.943212000
1	5.291802000	2.653471000	2.396864000
1	6.956342000	1.352333000	0.964431000
1	2.825605000	-0.943732000	2.082452000
6	4.418490000	0.270920000	1.270237000
1	5.636370000	-3.131554000	-0.328691000
6	6.065938000	-1.017931000	-0.133825000
6	3.443943000	-0.915536000	1.172879000
6	5.081311000	-2.188857000	-0.229898000
1	3.044726000	1.571399000	2.320585000
6	4.656406000	2.775088000	1.510261000
6	6.291124000	1.496978000	0.102446000
6	3.663086000	1.607933000	1.413229000
6	5.316477000	0.313491000	0.005081000
1	6.704213000	-0.987408000	-1.027362000

6	2.299509000	-3.230836000	-0.284494000
1	4.112908000	3.720870000	1.631176000
6	5.524374000	2.822329000	0.240777000
1	6.928572000	1.519725000	-0.791747000
1	1.588596000	-4.063221000	-0.352185000
1	6.235067000	3.654855000	0.308803000
1	0.896559000	-1.931626000	0.750564000
6	2.506233000	-0.721583000	-0.048344000
1	3.709923000	-4.128323000	-1.676431000
6	4.159679000	-2.015126000	-1.457335000
6	1.532171000	-1.906452000	-0.144191000
6	3.166559000	-3.182627000	-1.554295000
1	1.121214000	0.584211000	0.982661000
6	2.742571000	1.781636000	0.185273000
6	4.378739000	0.507518000	-1.216362000
6	1.759561000	0.610847000	0.090812000
6	3.403782000	-0.678759000	-1.313610000
1	4.777016000	-1.978212000	-2.365350000
6	4.617122000	3.012725000	-0.987219000
1	2.184990000	2.722974000	0.284027000
6	3.623647000	1.845449000	-1.081209000
1	4.996672000	0.535071000	-2.126216000
1	0.864144000	-1.763359000	-1.004551000
1	2.530381000	-3.060320000	-2.440266000
1	4.072986000	3.962766000	-0.910637000
1	1.093074000	0.748259000	-0.771433000
1	5.224387000	3.062383000	-1.900097000
1	2.756791000	-0.536302000	-2.192061000
1	2.977405000	1.979067000	-1.959609000

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6	2.574850000	1.778797000	-1.467360000
6	1.601129000	0.889416000	-0.664481000
6	1.788408000	1.192063000	0.838261000
6	2.305152000	3.263482000	-1.181316000
6	3.940326000	3.189984000	0.719065000
6	1.519872000	2.676131000	1.127003000
6	2.498807000	3.544936000	0.318883000
6	1.875979000	-0.591616000	-0.945025000
6	4.309170000	-0.076978000	-1.345166000
6	3.310629000	-0.962391000	-0.553773000
6	3.525180000	-0.662792000	0.953678000
6	4.966496000	-1.035547000	1.354875000
6	5.941711000	-0.146465000	0.551951000
6	5.752860000	-0.448275000	-0.951144000
6	4.016642000	1.407556000	-1.066521000
6	5.666711000	1.334999000	0.835510000
6	3.232594000	0.821655000	1.232125000
6	4.231708000	1.707353000	0.440866000
6	3.598861000	-2.445315000	-0.831854000

6	5.232455000	-2.521012000	1.069065000
6	6.019310000	-1.933298000	-1.239473000
6	5.039532000	-2.801899000	-0.431330000
1	2.441042000	1.578005000	-2.539184000
1	0.571920000	1.135196000	-0.956738000
1	1.092194000	0.572260000	1.417907000
1	2.985758000	3.888747000	-1.773221000
1	1.282943000	3.523727000	-1.484786000
1	4.099730000	3.399962000	1.785323000
1	4.652578000	3.813070000	0.161458000
1	1.635769000	2.874967000	2.200109000
1	0.484796000	2.928569000	0.864459000
1	2.309186000	4.605511000	0.523952000
1	1.174277000	-1.218166000	-0.381360000
1	1.714855000	-0.812304000	-2.009095000
1	4.168832000	-0.271792000	-2.418845000
1	2.820371000	-1.278634000	1.532232000
1	5.100226000	-0.835228000	2.426772000
1	6.972404000	-0.393046000	0.840686000
1	6.450356000	0.171952000	-1.530592000
1	4.720127000	2.023736000	-1.646039000
1	6.374752000	1.963395000	0.278279000
1	5.820863000	1.550015000	1.901692000
1	3.372283000	1.016480000	2.305871000
1	2.884788000	-3.066486000	-0.274043000
1	3.438407000	-2.655173000	-1.897942000
1	4.548775000	-3.144014000	1.659891000
1	6.253109000	-2.784895000	1.374236000
1	5.902842000	-2.132932000	-2.312383000
1	7.053979000	-2.186891000	-0.975497000
1	5.228708000	-3.862471000	-0.636793000
1	-6.549182000	-0.019981000	1.302159000
1	-4.830281000	-1.830858000	1.761604000
1	-6.058309000	2.365925000	1.840242000
1	-6.345951000	-2.012979000	-0.268968000
1	-7.110486000	2.250930000	0.427857000
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6	-6.097518000	2.039019000	0.793262000
1	-3.110375000	-3.653277000	2.229960000
1	-4.634498000	-3.822833000	0.188568000
1	-4.337489000	0.544755000	2.291367000
6	-4.088012000	-1.282051000	1.163065000
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1	-2.619779000	-1.263559000	2.752346000
6	-2.388911000	-3.097117000	1.617815000
6	-3.885189000	-3.263621000	-0.387849000
6	-2.677444000	-1.591340000	1.705352000

6	-4.196291000	-1.761177000	-0.308975000
1	-5.677169000	-1.792453000	-1.886797000
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1	-5.265037000	3.889180000	0.022684000
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6	-3.346571000	1.015861000	0.423753000
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6	-3.653772000	2.518857000	0.501175000
6	-5.147186000	2.354195000	-1.506853000
1	-1.864034000	1.046693000	2.001364000
6	-1.648871000	-0.795419000	0.872682000
6	-3.144069000	-0.967410000	-1.127464000
6	-1.944012000	0.705593000	0.960186000
6	-3.453310000	0.537050000	-1.048687000
1	-4.917829000	0.519911000	-2.640494000
6	-1.442075000	-2.780012000	-0.683295000
1	-0.641443000	-0.997985000	1.260135000
6	-1.731813000	-1.274931000	-0.593056000
1	-3.207449000	-1.289071000	-2.177692000
1	-2.901424000	3.074976000	-0.074634000
1	-4.422693000	2.907825000	-2.117778000
1	-0.428068000	-2.990448000	-0.319649000
1	-1.201607000	1.270813000	0.384090000
1	-1.480459000	-3.106249000	-1.730445000
1	-2.708404000	1.084638000	-1.645387000
1	-0.999705000	-0.721296000	-1.193882000

#### D4

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6	-4.481355000	3.055867000	0.613159000
6	-3.705982000	2.274791000	-1.640352000
6	-2.049871000	3.181917000	0.006921000
6	-3.485112000	3.315126000	-0.530320000
6	-2.614913000	0.078292000	2.275328000
6	-4.271885000	-0.837283000	0.611628000
6	-2.834484000	-0.973601000	1.180412000
6	-1.851860000	-0.709370000	0.010386000
6	-2.065311000	-1.763551000	-1.094256000
6	-3.501417000	-1.612658000	-1.641778000
6	-4.493571000	-1.892360000	-0.490945000
6	-4.480994000	0.587915000	0.071138000
6	-3.713174000	-0.199283000	-2.195634000
6	-2.060243000	0.715318000	-0.529323000

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6	-1.850322000	-3.177305000	-0.534748000
6	-4.280678000	-3.304924000	0.073136000
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1	-3.011430000	2.455240000	-2.471966000
1	-4.721880000	2.365194000	-2.047960000
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1	-1.595836000	-0.017548000	2.674891000
1	-3.303935000	-0.110847000	3.109641000
1	-4.986911000	-1.016379000	1.428373000
1	-0.828054000	-0.796538000	0.397774000
1	-1.351228000	-1.574658000	-1.908018000
1	-3.660541000	-2.350400000	-2.439822000
1	-5.519237000	-1.797030000	-0.872851000
1	-5.507889000	0.675078000	-0.313934000
1	-4.728902000	-0.101169000	-2.602271000
1	-3.018156000	-0.011552000	-3.025425000
1	-1.344373000	0.894407000	-1.345987000
1	-1.601303000	-2.484258000	2.119668000
1	-3.309006000	-2.578734000	2.555265000
1	-0.822376000	-3.285197000	-0.170398000
1	-1.988457000	-3.919982000	-1.330917000
1	-5.002910000	-3.499640000	0.876314000
1	-4.460465000	-4.052854000	-0.709642000
1	-2.690634000	-4.444863000	1.012465000
1	5.519217000	1.797038000	0.872888000
1	5.507871000	-0.675086000	0.314042000
1	5.002966000	3.499604000	-0.876344000
1	4.728806000	0.101231000	2.602328000
1	4.460468000	4.052865000	0.709578000
6	4.493566000	1.892365000	0.490942000
6	4.280704000	3.304915000	-0.073186000
1	5.510469000	-3.161085000	-0.246405000
1	4.721783000	-2.365149000	2.048086000
1	4.986969000	1.016325000	-1.428333000
6	4.480990000	-0.587926000	-0.071071000
1	3.660469000	2.350466000	2.439776000
6	3.713093000	0.199341000	2.195650000
6	4.271912000	0.837258000	-0.611609000
6	3.501369000	1.612702000	1.641746000
1	4.981827000	-1.455723000	-1.988493000
6	4.481351000	-3.055893000	-0.613022000

6	3.705901000	-2.274748000	1.640438000
6	4.267116000	-1.642721000	-1.175384000
6	3.496776000	-0.852175000	1.099915000
1	3.018043000	0.011639000	3.025421000
6	2.844881000	3.436524000	-0.609673000
1	4.345283000	-3.800431000	-1.407777000
6	3.485063000	-3.315112000	0.530427000
1	3.011316000	-2.455168000	2.472031000
1	2.690703000	4.444839000	-1.012605000
1	3.637948000	-4.323546000	0.933474000
1	3.309119000	2.578662000	-2.555330000
6	2.834533000	0.973571000	-1.180450000
1	1.988434000	3.920030000	1.330765000
6	2.065284000	1.763591000	1.094168000
6	2.620643000	2.396155000	-1.719235000
6	1.850325000	3.177331000	0.534612000
1	3.304050000	0.110760000	-3.109637000
6	2.830906000	-1.491735000	-1.722413000
6	2.060216000	-0.715293000	0.529303000
6	2.614995000	-0.078351000	-2.275345000
6	1.851864000	0.709381000	-0.010453000
1	1.351171000	1.574726000	1.907910000
6	2.049844000	-3.181907000	-0.006871000
1	2.670717000	-2.229386000	-2.520381000
6	1.839306000	-1.770386000	-0.572642000
1	1.344315000	-0.894354000	1.345947000
1	1.601399000	2.484212000	-2.119794000
1	0.822392000	3.285217000	0.170221000
1	1.865139000	-3.931236000	-0.787111000
1	1.595933000	0.017486000	-2.674949000
1	1.329144000	-3.373160000	0.798804000
1	0.828072000	0.796547000	-0.397880000
1	0.817014000	-1.674996000	-0.957600000

### D5

6	-5.081784000	1.227878000	-0.708117000
6	-5.015067000	1.147362000	0.832814000
6	-3.654384000	1.716871000	1.292041000
6	-4.920136000	2.681186000	-1.178885000
6	-2.435109000	2.366247000	-1.302259000
6	-3.491221000	3.170517000	0.824246000
6	-3.560736000	3.230504000	-0.711438000
6	-5.168490000	-0.306337000	1.296105000
6	-4.093367000	-1.114832000	-0.834543000
6	-4.051619000	-1.183311000	0.715259000
6	-2.674931000	-0.624461000	1.160390000
6	-1.548849000	-1.499872000	0.579745000
6	-1.611203000	-1.421086000	-0.961747000
6	-2.969598000	-1.994592000	-1.421648000
6	-3.957270000	0.348788000	-1.291239000

6	-1.466496000	0.029520000	-1.434574000
6	-2.534606000	0.836530000	0.702298000
6	-2.578823000	0.906046000	-0.847674000
6	-4.186761000	-2.643694000	1.173537000
6	-1.700307000	-2.952988000	1.049795000
6	-3.127183000	-3.448173000	-0.952061000
6	-3.058206000	-3.506389000	0.583711000
1	-6.051224000	0.835768000	-1.044893000
1	-5.822058000	1.758221000	1.259577000
1	-3.599998000	1.672756000	2.388421000
1	-4.989848000	2.729965000	-2.273106000
1	-5.734073000	3.298013000	-0.776944000
1	-1.455502000	2.751659000	-0.987537000
1	-2.457848000	2.411440000	-2.399441000
1	-2.530140000	3.569594000	1.173322000
1	-4.278499000	3.796918000	1.262745000
1	-3.445325000	4.268154000	-1.047195000
1	-5.140936000	-0.357528000	2.393075000
1	-6.144956000	-0.700556000	0.983301000
1	-5.065428000	-1.503740000	-1.172512000
1	-2.624915000	-0.658941000	2.258947000
1	-0.586432000	-1.103036000	0.923813000
1	-0.800664000	-2.030002000	-1.385518000
1	-3.021914000	-1.952379000	-2.518145000
1	-4.007456000	0.384598000	-2.389674000
1	-1.508093000	0.071908000	-2.531527000
1	-0.491151000	0.431761000	-1.140392000
1	-1.561743000	1.222554000	1.040604000
1	-4.161447000	-2.685685000	2.270800000
1	-5.164285000	-3.035842000	0.861984000
1	-1.627078000	-3.002031000	2.143765000
1	-0.882986000	-3.564527000	0.645393000
1	-4.085316000	-3.853210000	-1.302001000
1	-2.335726000	-4.070519000	-1.388968000
1	-3.171905000	-4.543767000	0.920820000
1	4.417227000	1.565688000	2.544568000
1	4.854080000	-0.810577000	1.766421000
1	5.135504000	3.514583000	1.162215000
1	2.729574000	-0.276539000	3.051151000
1	3.659238000	3.893353000	2.052335000
6	3.900160000	1.783378000	1.600009000
6	4.069258000	3.269048000	1.248187000
1	5.290338000	-3.200343000	0.995110000
1	3.152977000	-2.648248000	2.279053000
1	5.568317000	1.125139000	0.383892000
6	4.337771000	-0.598748000	0.818258000
1	1.970436000	2.048375000	2.553046000
6	2.236672000	-0.051349000	2.095607000
6	4.497230000	0.896427000	0.488263000
6	2.403927000	1.432960000	1.753053000

1	6.008343000	-1.254285000	-0.390800000
6	4.763176000	-2.971639000	0.060038000
6	2.665098000	-2.426557000	1.320280000
6	4.939161000	-1.486296000	-0.290763000
6	2.833429000	-0.935232000	0.992443000
1	1.172347000	-0.290626000	2.223926000
6	3.349521000	3.573674000	-0.077411000
1	5.210933000	-3.597009000	-0.722884000
6	3.266191000	-3.297355000	0.205205000
1	1.597883000	-2.654771000	1.445213000
1	3.471352000	4.634040000	-0.329533000
1	3.140504000	-4.357577000	0.456137000
1	5.019832000	2.939851000	-1.319334000
6	3.797263000	1.211799000	-0.860944000
1	1.403291000	3.867031000	0.851633000
6	1.689253000	1.757899000	0.423874000
6	3.954788000	2.703699000	-1.191412000
6	1.854002000	3.242325000	0.069806000
1	5.458951000	0.568292000	-2.089114000
6	4.227089000	-1.157825000	-1.621834000
6	2.137551000	-0.619950000	-0.357098000
6	4.394500000	0.327551000	-1.963594000
6	2.293591000	0.873340000	-0.685254000
1	0.622563000	1.521055000	0.527547000
6	2.549319000	-2.988669000	-1.120503000
1	4.661054000	-1.772537000	-2.422058000
6	2.730251000	-1.504540000	-1.470584000
1	1.072448000	-0.852369000	-0.255805000
1	3.463048000	2.918984000	-2.149673000
1	1.323296000	3.464627000	-0.865154000
1	2.953621000	-3.617071000	-1.924310000
1	3.902277000	0.551951000	-2.919679000
1	1.480403000	-3.224460000	-1.034328000
1	1.776744000	1.084923000	-1.633308000
1	2.212027000	-1.280950000	-2.413278000

### D6

6	-4.740610000	2.410437000	-0.670597000
6	-4.784060000	2.329218000	0.871175000
6	-3.377978000	1.940855000	1.379030000
6	-3.701713000	3.446523000	-1.124945000
6	-1.944091000	1.659081000	-1.170696000
6	-2.335177000	2.973575000	0.926176000
6	-2.309215000	3.042958000	-0.610510000
6	-5.817211000	1.289194000	1.320104000
6	-5.412799000	-0.040493000	-0.780886000
6	-5.467247000	-0.099367000	0.768898000
6	-4.054055000	-0.508608000	1.262033000
6	-3.696140000	-1.903323000	0.709533000
6	-3.655202000	-1.822236000	-0.832349000

6	-5.061272000	-1.434538000	-1.339297000
6	-4.384057000	1.015006000	-1.222354000
6	-2.622022000	-0.783338000	-1.280627000
6	-3.026622000	0.547174000	0.821063000
6	-2.971059000	0.605343000	-0.728865000
6	-6.493951000	-1.152953000	1.211403000
6	-4.733963000	-2.939425000	1.165540000
6	-6.101066000	-2.469685000	-0.885572000
6	-6.127276000	-2.537040000	0.651228000
1	-5.734453000	2.695943000	-1.041679000
1	-5.052159000	3.314917000	1.275000000
1	-3.395607000	1.889750000	2.476301000
1	-3.693453000	3.513142000	-2.220403000
1	-3.971520000	4.439880000	-0.744153000
1	-0.945776000	1.365533000	-0.822946000
1	-1.901765000	1.691639000	-2.267860000
1	-1.343736000	2.695475000	1.306695000
1	-2.575891000	3.959103000	1.344751000
1	-1.565297000	3.780485000	-0.935372000
1	-5.858862000	1.247982000	2.417063000
1	-6.818719000	1.578908000	0.974049000
1	-6.405970000	0.254148000	-1.151374000
1	-4.069806000	-0.551891000	2.361249000
1	-2.700980000	-2.187132000	1.078723000
1	-3.386559000	-2.807827000	-1.236134000
1	-5.043962000	-1.383591000	-2.436589000
1	-4.367526000	1.057620000	-2.321601000
1	-2.578371000	-0.741392000	-2.377507000
1	-1.624472000	-1.077369000	-0.934046000
1	-2.035408000	0.253376000	1.195143000
1	-6.533162000	-1.186415000	2.308582000
1	-7.493622000	-0.857126000	0.865577000
1	-4.741375000	-3.005026000	2.261082000
1	-4.464148000	-3.933056000	0.785523000
1	-7.093086000	-2.196569000	-1.267573000
1	-5.855864000	-3.454899000	-1.302414000
1	-6.869610000	-3.275729000	0.976965000
1	2.592945000	0.758179000	-2.412150000
1	5.092738000	0.916809000	-2.025068000
1	1.488180000	-1.466542000	-2.655336000
1	3.538003000	2.599222000	-0.930042000
1	0.394473000	-0.304604000	-1.906158000
6	2.495464000	0.098466000	-1.539131000
6	1.321458000	-0.868082000	-1.750513000
1	7.605900000	1.083206000	-1.649788000
1	6.032679000	2.763740000	-0.546617000
1	3.989138000	-1.295304000	-2.258631000
6	5.003648000	0.257156000	-1.149093000
1	1.342452000	1.541593000	-0.402271000
6	3.447646000	1.919798000	-0.071616000

6	3.808937000	-0.688669000	-1.358654000
6	2.268011000	0.963179000	-0.279499000
1	6.489859000	-1.135893000	-1.877453000
6	7.495301000	0.434869000	-0.771151000
6	5.949292000	2.085094000	0.312984000
6	6.318375000	-0.530110000	-0.977112000
6	4.756937000	1.139283000	0.103697000
1	3.273349000	2.546528000	0.813592000
6	1.185604000	-1.791824000	-0.527673000
1	8.430504000	-0.130322000	-0.668676000
6	7.251685000	1.286698000	0.486640000
1	5.768147000	2.711217000	1.197072000
1	0.344999000	-2.481063000	-0.675787000
1	8.091024000	1.976905000	0.634816000
1	2.668692000	-3.217836000	-1.235824000
6	3.679968000	-1.644984000	-0.143043000
1	0.010350000	-0.374919000	0.630375000
6	2.119269000	0.024040000	0.937549000
6	2.487120000	-2.591109000	-0.352322000
6	0.943438000	-0.941016000	0.730820000
1	5.162558000	-3.052833000	-0.853053000
6	6.169069000	-1.469678000	0.239737000
6	4.628926000	0.183149000	1.319371000
6	4.988877000	-2.425951000	0.032157000
6	3.434034000	-0.762804000	1.110010000
1	1.945990000	0.630119000	1.837422000
6	7.119055000	0.360425000	1.707893000
1	7.095321000	-2.047098000	0.362937000
6	5.942547000	-0.604491000	1.499114000
1	4.448701000	0.789694000	2.219426000
1	2.403122000	-3.268841000	0.507930000
1	0.830890000	-1.590348000	1.608602000
1	8.047503000	-0.206267000	1.854153000
1	4.898233000	-3.105297000	0.890652000
1	6.958741000	0.955182000	2.616269000
1	3.344559000	-1.422450000	1.985950000
1	5.844866000	-1.263458000	2.372710000

### D7

6	-4.400535000	-2.190279000	0.130669000
6	-3.943218000	-1.888451000	-1.313806000
6	-2.399588000	-1.839560000	-1.335196000
6	-3.814035000	-3.525724000	0.612712000
6	-1.805538000	-2.320674000	1.504520000
6	-1.811753000	-3.175044000	-0.855708000
6	-2.277088000	-3.457682000	0.583393000
6	-4.524924000	-0.551481000	-1.787713000
6	-4.505269000	0.312376000	0.579047000
6	-4.061037000	0.595983000	-0.881214000
6	-2.511028000	0.659493000	-0.882204000

6	-2.040451000	1.809922000	0.028708000
6	-2.496124000	1.510306000	1.472973000
6	-4.039816000	1.463350000	1.494606000
6	-3.931052000	-1.038098000	1.042234000
6	-1.916883000	0.173154000	1.948765000
6	-1.937879000	-0.689636000	-0.418406000
6	-2.380613000	-0.973546000	1.041176000
6	-4.633527000	1.944165000	-1.344505000
6	-2.620335000	3.146315000	-0.454531000
6	-4.625113000	2.799188000	1.012728000
6	-4.157291000	3.081509000	-0.425758000
1	-5.497845000	-2.238124000	0.155270000
1	-4.286290000	-2.695919000	-1.974739000
1	-2.061029000	-1.633463000	-2.359987000
1	-4.162158000	-3.741446000	1.630975000
1	-4.167639000	-4.343440000	-0.028245000
1	-0.708879000	-2.268149000	1.513631000
1	-2.122052000	-2.515938000	2.538039000
1	-0.716053000	-3.141131000	-0.899615000
1	-2.133670000	-3.986199000	-1.521256000
1	-1.856793000	-4.410259000	0.927903000
1	-4.213262000	-0.350104000	-2.821675000
1	-5.622514000	-0.596935000	-1.789024000
1	-5.603901000	0.258279000	0.602116000
1	-2.170638000	0.855021000	-1.910298000
1	-0.945821000	1.855405000	0.003137000
1	-2.150937000	2.318172000	2.132528000
1	-4.377443000	1.260029000	2.520097000
1	-4.269196000	-1.234200000	2.070669000
1	-2.232413000	-0.027636000	2.981656000
1	-0.819626000	0.216366000	1.955655000
1	-0.842530000	-0.633389000	-0.442371000
1	-4.320615000	2.137196000	-2.379533000
1	-5.730769000	1.894116000	-1.347292000
1	-2.269683000	3.359636000	-1.472576000
1	-2.263734000	3.963353000	0.185843000
1	-5.721364000	2.763476000	1.051836000
1	-4.305697000	3.610496000	1.679261000
1	-4.575562000	4.034771000	-0.770905000
1	4.377448000	-1.260027000	-2.520096000
1	4.269200000	1.234201000	-2.070666000
1	5.721366000	-2.763475000	-1.051834000
1	2.232418000	0.027638000	-2.981658000
1	4.305700000	-3.610495000	-1.679262000
6	4.039819000	-1.463349000	-1.494606000
6	4.625115000	-2.799187000	-1.012727000
1	4.162160000	3.741447000	-1.630970000
1	2.122056000	2.515940000	-2.538039000
1	5.603902000	-0.258278000	-0.602112000
6	3.931054000	1.038098000	-1.042232000

1	2.150941000	-2.318171000	-2.132531000
6	1.916887000	-0.173153000	-1.948768000
6	4.505270000	-0.312375000	-0.579046000
6	2.496127000	-1.510305000	-1.472976000
1	5.497845000	2.238125000	-0.155264000
6	3.814036000	3.525725000	-0.612709000
6	1.805541000	2.320675000	-1.504521000
6	4.400535000	2.190279000	-0.130665000
6	2.380615000	0.973547000	-1.041177000
1	0.819629000	-0.216365000	-1.955660000
6	4.157291000	-3.081509000	0.425758000
1	4.167638000	4.343440000	0.028249000
6	2.277089000	3.457683000	-0.583393000
1	0.708881000	2.268150000	-1.513634000
1	4.575561000	-4.034771000	0.770904000
1	1.856794000	4.410260000	-0.927902000
1	5.730767000	-1.894117000	1.347295000
6	4.061036000	-0.595984000	0.881215000
1	2.263735000	-3.963353000	-0.185848000
6	2.040451000	-1.809922000	-0.028711000
6	4.633525000	-1.944166000	1.344506000
6	2.620334000	-3.146315000	0.454528000
1	5.622510000	0.596934000	1.789029000
6	3.943215000	1.888450000	1.313808000
6	1.937879000	0.689636000	0.418404000
6	4.524921000	0.551480000	1.787715000
6	2.511026000	-0.659493000	0.882202000
1	0.945821000	-1.855405000	-0.003143000
6	1.811751000	3.175044000	0.855708000
1	4.286286000	2.695917000	1.974743000
6	2.399585000	1.839559000	1.335196000
1	0.842529000	0.633388000	0.442366000
1	4.320610000	-2.137198000	2.379533000
1	2.269680000	-3.359637000	1.472572000
1	2.133667000	3.986198000	1.521257000
1	4.213257000	0.350102000	2.821677000
1	0.716051000	3.141130000	0.899612000
1	2.170635000	-0.855022000	1.910296000
1	2.061024000	1.633461000	2.359986000

### D8

6	4.602438000	-1.846625000	0.068515000
6	4.047098000	-1.532018000	1.475443000
6	2.510103000	-1.676465000	1.435269000
6	4.207621000	-3.267478000	-0.361881000
6	2.106014000	-2.370288000	-1.392507000
6	2.115209000	-3.097939000	1.009650000
6	2.673830000	-3.391737000	-0.393024000
6	4.436978000	-0.110250000	1.896002000
6	4.417928000	0.623970000	-0.514637000

6	3.875447000	0.922547000	0.909299000
6	2.330815000	0.790639000	0.846403000
6	1.765483000	1.825683000	-0.146476000
6	2.320454000	1.511991000	-1.552303000
6	3.857706000	1.658970000	-1.512120000
6	4.036044000	-0.809946000	-0.923738000
6	1.929507000	0.090358000	-1.971108000
6	1.949948000	-0.641388000	0.438410000
6	2.491747000	-0.940975000	-0.984675000
6	4.256011000	2.353815000	1.317742000
6	2.153268000	3.247196000	0.282582000
6	4.250569000	3.080642000	-1.083384000
6	3.686252000	3.374831000	0.318110000
1	5.697359000	-1.757348000	0.088661000
1	4.457590000	-2.255638000	2.192629000
1	2.102928000	-1.462942000	2.433284000
1	4.624369000	-3.487413000	-1.353204000
1	4.630629000	-4.002085000	0.335198000
1	1.012187000	-2.452949000	-1.442199000
1	2.486328000	-2.577463000	-2.401838000
1	1.023824000	-3.200237000	1.011951000
1	2.507832000	-3.827174000	1.730071000
1	2.389744000	-4.405763000	-0.699491000
1	4.056174000	0.102087000	2.904444000
1	5.530531000	-0.016757000	1.942012000
1	5.514908000	0.706587000	-0.490930000
1	1.922028000	0.995396000	1.847173000
1	0.671478000	1.734687000	-0.168152000
1	1.908050000	2.235429000	-2.269214000
1	4.265370000	1.447539000	-2.510136000
1	4.441843000	-1.013625000	-1.925897000
1	2.307447000	-0.123362000	-2.980123000
1	0.837318000	-0.008662000	-2.010676000
1	0.855664000	-0.724168000	0.415893000
1	3.874442000	2.558852000	2.327177000
1	5.349779000	2.441213000	1.366328000
1	1.732223000	3.466721000	1.272181000
1	1.728101000	3.978712000	-0.416586000
1	5.343652000	3.181041000	-1.077709000
1	3.864258000	3.810457000	-1.806188000
1	3.968040000	4.389316000	0.624825000
1	-5.427260000	1.596859000	-1.321497000
1	-5.313622000	-0.897412000	-0.854195000
1	-5.458958000	3.247688000	0.549456000
1	-4.123654000	0.057863000	-2.884568000
1	-4.630104000	3.917231000	-0.857613000
6	-4.522877000	1.752970000	-0.717651000
6	-4.563100000	3.148796000	-0.076860000
1	-5.214585000	-3.397908000	-0.387085000
1	-4.012081000	-2.425067000	-2.424510000

1	-5.347685000	0.740646000	1.011399000
6	-4.408594000	-0.745303000	-0.247215000
1	-3.326026000	2.375557000	-2.414847000
6	-3.235748000	0.217719000	-2.258159000
6	-4.455991000	0.663386000	0.371762000
6	-3.281103000	1.612861000	-1.625717000
1	-5.235625000	-1.747037000	1.482967000
6	-4.304679000	-3.229104000	0.202806000
6	-3.124813000	-2.273335000	-1.795139000
6	-4.346666000	-1.833974000	0.843423000
6	-3.170963000	-0.867849000	-1.176318000
1	-2.360452000	0.130774000	-2.916950000
6	-3.298943000	3.366618000	0.773071000
1	-4.279744000	-3.999713000	0.983815000
6	-3.062352000	-3.347877000	-0.697265000
1	-2.248605000	-2.353429000	-2.452703000
1	-3.328278000	4.362469000	1.231667000
1	-3.030780000	-4.343472000	-1.155998000
1	-4.110338000	2.377618000	2.533400000
6	-3.198920000	0.886755000	1.253190000
1	-2.075880000	4.015932000	-0.905858000
6	-2.020786000	1.850060000	-0.766397000
6	-3.238099000	2.292358000	1.871458000
6	-2.055345000	3.244424000	-0.125698000
1	-4.002182000	-0.113524000	2.997234000
6	-3.085346000	-1.594884000	1.701603000
6	-1.914876000	-0.642773000	-0.294977000
6	-3.130041000	-0.199372000	2.334781000
6	-1.963201000	0.762242000	0.324300000
1	-1.133697000	1.760574000	-1.407916000
6	-1.798392000	-3.126479000	0.149691000
1	-3.038410000	-2.357353000	2.491000000
6	-1.843747000	-1.732936000	0.793085000
1	-1.021155000	-0.705448000	-0.931117000
1	-2.347226000	2.439825000	2.496658000
1	-1.144078000	3.407585000	0.463942000
1	-1.722632000	-3.897444000	0.927286000
1	-2.239473000	-0.039513000	2.957535000
1	-0.906385000	-3.218094000	-0.481182000
1	-1.060247000	0.909322000	0.935854000
1	-0.940265000	-1.576005000	1.398268000

**Table S6.** Geometries in Cartesian coordinates in Å computed at the M06-2X/6-31G(d,p) level of theory.

<b>1</b>			
6	-1.457309000	-1.301791000	1.250996000
6	-2.180160000	-0.763799000	0.000000000
6	-1.457309000	-1.301791000	-1.250996000

6	-1.457309000	-2.835216000	1.251716000
6	0.710381000	-2.833751000	0.0000000000
6	-1.457309000	-2.835216000	-1.251716000
6	-0.733849000	-3.352348000	0.0000000000
6	-2.170552000	0.767345000	0.0000000000
6	0.013138000	0.768295000	1.247446000
6	-0.734460000	1.300421000	0.0000000000
6	0.013138000	0.768295000	-1.247446000
6	1.457309000	1.301791000	-1.250996000
6	2.180160000	0.763799000	0.0000000000
6	1.457309000	1.301791000	1.250996000
6	-0.013138000	-0.768295000	1.247446000
6	2.170552000	-0.767345000	0.0000000000
6	-0.013138000	-0.768295000	-1.247446000
6	0.734460000	-1.300421000	0.0000000000
6	-0.710381000	2.833751000	0.0000000000
6	1.457309000	2.835216000	-1.251716000
6	1.457309000	2.835216000	1.251716000
6	0.733849000	3.352348000	0.0000000000
1	-1.971289000	-0.929365000	2.148327000
1	-3.216392000	-1.129824000	0.0000000000
1	-1.971289000	-0.929365000	-2.148327000
1	-0.958480000	-3.208261000	2.155291000
1	-2.488768000	-3.209552000	1.271204000
1	1.246905000	-3.205954000	-0.883937000
1	1.246905000	-3.205954000	0.883937000
1	-0.958480000	-3.208261000	-2.155291000
1	-2.488768000	-3.209552000	-1.271204000
1	-0.732564000	-4.448526000	0.0000000000
1	-2.700810000	1.148630000	-0.883998000
1	-2.700810000	1.148630000	0.883998000
1	-0.508899000	1.135401000	2.145770000
1	-0.508899000	1.135401000	-2.145770000
1	1.971289000	0.929365000	-2.148327000
1	3.216392000	1.129824000	0.0000000000
1	1.971289000	0.929365000	2.148327000
1	0.508899000	-1.135401000	2.145770000
1	2.700810000	-1.148630000	0.883998000
1	2.700810000	-1.148630000	-0.883998000
1	0.508899000	-1.135401000	-2.145770000
1	-1.246905000	3.205954000	-0.883937000
1	-1.246905000	3.205954000	0.883937000
1	0.958480000	3.208261000	-2.155291000
1	2.488768000	3.209552000	-1.271204000
1	0.958480000	3.208261000	2.155291000
1	2.488768000	3.209552000	1.271204000
1	0.732564000	4.448526000	0.0000000000

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**D1**

6	-4.864352000	-0.886983000	-0.951024000
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6	-3.557245000	-1.117183000	-1.735434000
6	-2.514491000	-1.728653000	-0.778716000
6	-5.380848000	-2.209300000	-0.371351000
6	-4.057359000	-1.808829000	1.715349000
6	-3.029520000	-3.051344000	-0.199021000
6	-4.330222000	-2.802598000	0.578361000
6	-3.039030000	0.206045000	-2.305224000
6	-4.065111000	1.453465000	-0.376435000
6	-2.764757000	1.210191000	-1.181598000
6	-1.721893000	0.614878000	-0.203718000
6	-1.441322000	1.620833000	0.926833000
6	-2.748237000	1.850773000	1.711844000
6	-3.791398000	2.461465000	0.754574000
6	-4.583665000	0.118383000	0.180394000
6	-3.263136000	0.526161000	2.281832000
6	-2.240145000	-0.720414000	0.352027000
6	-3.540172000	-0.477225000	1.158006000
6	-2.246293000	2.541208000	-1.739147000
6	-0.923943000	2.941393000	0.344249000
6	-3.276410000	3.784338000	0.175048000
6	-1.975997000	3.536058000	-0.602538000
1	-5.616729000	-0.458621000	-1.628176000
1	-3.750273000	-1.824691000	-2.553871000
1	-1.581828000	-1.904059000	-1.334127000
1	-6.321411000	-2.038704000	0.167801000
1	-5.594808000	-2.915608000	-1.183605000
1	-3.315534000	-2.224141000	2.411795000
1	-4.976200000	-1.629794000	2.291042000
1	-2.273214000	-3.489444000	0.465575000
1	-3.205814000	-3.770882000	-1.008722000
1	-4.699023000	-3.747412000	0.994104000
1	-2.113506000	0.035190000	-2.873621000
1	-3.773679000	0.631320000	-3.003384000
1	-4.820667000	1.874342000	-1.059248000
1	-0.789413000	0.433043000	-0.763109000
1	-0.688779000	1.192225000	1.606340000
1	-2.555151000	2.558405000	2.530167000
1	-4.724703000	2.636052000	1.308251000
1	-5.515413000	0.301178000	0.739612000
1	-4.185491000	0.694645000	2.855305000
1	-2.524439000	0.100900000	2.975837000
1	-1.484530000	-1.141144000	1.037662000
1	-1.324634000	2.360721000	-2.310671000
1	-2.985361000	2.955547000	-2.438999000
1	0.011575000	2.764963000	-0.202670000
1	-0.697758000	3.647683000	1.154008000
1	-4.033450000	4.221371000	-0.488488000
1	-3.098688000	4.503577000	0.984672000
1	-1.607028000	4.480832000	-1.018213000
1	4.724692000	-2.636037000	-1.308290000

1	5.515406000	-0.301167000	-0.739633000
1	4.033457000	-4.221376000	0.488438000
1	4.185463000	-0.694614000	-2.855319000
1	3.098681000	-4.503566000	-0.984716000
6	3.791393000	-2.461457000	-0.754602000
6	3.276411000	-3.784336000	-0.175086000
1	6.321407000	2.038708000	-0.167805000
1	4.976177000	1.629821000	-2.291038000
1	4.820678000	-1.874351000	1.059217000
6	4.583663000	-0.118379000	-0.180404000
1	2.555128000	-2.558378000	-2.530185000
6	3.263114000	-0.526136000	-2.281835000
6	4.065115000	-1.453468000	0.376414000
6	2.748222000	-1.850755000	-1.711856000
1	5.616743000	0.458606000	1.628163000
6	5.380849000	2.209298000	0.371358000
6	4.057341000	1.808848000	-1.715334000
6	4.864360000	0.886975000	0.951021000
6	3.540161000	0.477238000	-1.158001000
1	2.524410000	-0.100869000	-2.975829000
6	1.976006000	-3.536066000	0.602516000
1	5.594816000	2.915597000	1.183617000
6	4.330214000	2.802605000	-0.578338000
1	3.315508000	2.224167000	-2.411769000
1	1.607042000	-4.480845000	1.018184000
1	4.699010000	3.747424000	-0.994075000
1	2.985388000	-2.955571000	2.438973000
6	2.764769000	-1.210204000	1.181593000
1	0.697748000	-3.647672000	-1.154018000
6	1.441315000	-1.620825000	-0.926830000
6	2.246312000	-2.541227000	1.739133000
6	0.923942000	-2.941390000	-0.344254000
1	3.773708000	-0.631350000	3.003376000
6	3.557259000	1.117165000	1.735445000
6	2.240141000	0.720417000	-0.352008000
6	3.039051000	-0.206069000	2.305227000
6	1.721895000	-0.614881000	0.203729000
1	0.688765000	-1.192211000	-1.606327000
6	3.029519000	3.051342000	0.199057000
1	3.750294000	1.824665000	2.553887000
6	2.514496000	1.728644000	0.778743000
1	1.484520000	1.141152000	-1.037632000
1	1.324659000	-2.360748000	2.310669000
1	-0.011569000	-2.764966000	0.202678000
1	3.205819000	3.770871000	1.008764000
1	2.113533000	-0.035221000	2.873634000
1	2.273207000	3.489449000	-0.465527000
1	0.789420000	-0.433052000	0.763131000
1	1.581836000	1.904043000	1.334164000

<b>D2</b>			
6	-3.196864000	-1.828424000	-0.847472000
6	-2.643903000	-1.643775000	0.579469000
6	-3.832654000	-1.536819000	1.555307000
6	-4.067634000	-3.087953000	-0.925915000
6	-6.081300000	-1.730613000	-0.319475000
6	-4.703767000	-2.796316000	1.478316000
6	-5.245593000	-2.963087000	0.051336000
6	-1.783083000	-0.380442000	0.648925000
6	-3.173452000	0.694847000	-1.142891000
6	-2.604071000	0.860167000	0.287510000
6	-3.807954000	0.985057000	1.252995000
6	-4.636252000	2.230049000	0.886358000
6	-5.189061000	2.045721000	-0.540965000
6	-3.999629000	1.938970000	-1.516213000
6	-4.024787000	-0.582788000	-1.214012000
6	-6.050730000	0.782118000	-0.616000000
6	-4.659256000	-0.292422000	1.181889000
6	-5.229197000	-0.457628000	-0.248403000
6	-1.750450000	2.132490000	0.357615000
6	-3.765185000	3.489522000	0.965426000
6	-3.128694000	3.198665000	-1.438386000
6	-2.586799000	3.365231000	-0.011308000
1	-2.353463000	-1.914253000	-1.547592000
1	-2.037115000	-2.521513000	0.844716000
1	-3.446523000	-1.413148000	2.576926000
1	-4.440874000	-3.221418000	-1.949290000
1	-3.467494000	-3.973268000	-0.680061000
1	-6.937340000	-1.633702000	0.362841000
1	-6.488000000	-1.839815000	-1.334567000
1	-5.535813000	-2.719260000	2.189789000
1	-4.113721000	-3.677231000	1.761628000
1	-5.869338000	-3.862749000	-0.004621000
1	-1.362198000	-0.261690000	1.658523000
1	-0.935881000	-0.466723000	-0.044560000
1	-2.326373000	0.600701000	-1.841762000
1	-3.418925000	1.099667000	2.277590000
1	-5.478509000	2.315823000	1.587325000
1	-5.792888000	2.924439000	-0.807448000
1	-4.385488000	1.816137000	-2.538037000
1	-4.413923000	-0.697297000	-2.238563000
1	-6.457746000	0.661962000	-1.629864000
1	-6.907021000	0.867574000	0.067733000
1	-5.505007000	-0.198529000	1.882022000
1	-1.339414000	2.240344000	1.371695000
1	-0.895770000	2.035712000	-0.326936000
1	-3.392531000	3.622226000	1.989107000
1	-4.364908000	4.375239000	0.719868000
1	-2.296596000	3.121949000	-2.149816000
1	-3.718929000	4.079544000	-1.721464000

1	-1.963343000	4.265079000	0.044844000
1	4.833780000	-2.295079000	2.015598000
1	4.994687000	0.225956000	2.173355000
1	2.613774000	-3.427134000	1.920487000
1	6.724896000	-1.063276000	0.852838000
1	3.815438000	-4.333228000	0.993810000
6	4.212567000	-2.204738000	1.113395000
6	3.248631000	-3.394003000	1.025928000
1	5.157693000	2.754492000	2.343375000
1	6.888870000	1.445348000	1.012850000
1	2.775490000	-0.895529000	2.071128000
6	4.371033000	0.325185000	1.270353000
1	5.705924000	-3.098016000	-0.175506000
6	6.085516000	-0.970079000	-0.036275000
6	3.425539000	-0.883032000	1.181454000
6	5.130133000	-2.163297000	-0.124823000
1	2.936590000	1.625510000	2.232316000
6	4.548738000	2.835350000	1.433951000
6	6.250668000	1.549566000	0.124274000
6	3.584228000	1.646765000	1.344521000
6	5.304732000	0.345937000	0.035057000
1	6.750123000	-0.952447000	-0.911509000
6	2.377995000	-3.262258000	-0.232028000
1	3.982052000	3.772568000	1.503869000
6	5.454811000	2.859691000	0.194561000
1	6.914677000	1.555846000	-0.751408000
1	1.687521000	-4.111300000	-0.294610000
1	6.145493000	3.708535000	0.257762000
1	0.919580000	-1.959067000	0.719211000
6	2.527451000	-0.748358000	-0.072970000
1	3.848931000	-4.174184000	-1.543698000
6	4.247421000	-2.048366000	-1.383662000
6	1.581316000	-1.952676000	-0.159173000
6	3.282590000	-3.236839000	-1.472504000
1	1.080244000	0.554817000	0.869955000
6	2.702723000	1.761961000	0.084794000
6	4.406909000	0.480839000	-1.219580000
6	1.748914000	0.568413000	-0.002831000
6	3.460753000	-0.727191000	-1.308752000
1	4.893932000	-2.027146000	-2.272311000
6	4.585865000	2.991735000	-1.064479000
1	2.123877000	2.695309000	0.135563000
6	3.620990000	1.803331000	-1.152633000
1	5.056823000	0.492533000	-2.109398000
1	0.938036000	-1.849691000	-1.045663000
1	2.672572000	-3.155349000	-2.381161000
1	4.019794000	3.931430000	-1.033584000
1	1.110192000	0.659798000	-0.894299000
1	5.221778000	3.023889000	-1.958361000
1	2.836665000	-0.627449000	-2.211431000

1	3.000469000	1.894034000	-2.055299000
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**D3**

6	2.548182000	1.775501000	-1.460192000
6	1.577349000	0.903510000	-0.639783000
6	1.785095000	1.213449000	0.855988000
6	2.297510000	3.262335000	-1.180738000
6	3.952478000	3.184577000	0.696234000
6	1.536373000	2.700172000	1.136537000
6	2.512702000	3.551148000	0.311999000
6	1.834108000	-0.581345000	-0.909303000
6	4.262419000	-0.092854000	-1.347246000
6	3.269124000	-0.960632000	-0.536207000
6	3.504826000	-0.655318000	0.963393000
6	4.946058000	-1.036809000	1.347121000
6	5.916847000	-0.164937000	0.525912000
6	5.705467000	-0.473245000	-0.969892000
6	3.988693000	1.394660000	-1.075143000
6	5.658698000	1.318867000	0.803074000
6	3.229003000	0.832232000	1.234798000
6	4.224090000	1.699844000	0.424610000
6	3.538717000	-2.445437000	-0.808187000
6	5.194359000	-2.524035000	1.067580000
6	5.953801000	-1.960297000	-1.250467000
6	4.978514000	-2.812217000	-0.425182000
1	2.399094000	1.567245000	-2.529056000
1	0.545947000	1.159587000	-0.923636000
1	1.087232000	0.603216000	1.448034000
1	2.978274000	3.875764000	-1.784594000
1	1.273444000	3.529930000	-1.471180000
1	4.126783000	3.397596000	1.760168000
1	4.664718000	3.795044000	0.123708000
1	1.668576000	2.905204000	2.206538000
1	0.500581000	2.961612000	0.881718000
1	2.336509000	4.614413000	0.511934000
1	1.136134000	-1.195042000	-0.322018000
1	1.654044000	-0.813866000	-1.969022000
1	4.103983000	-0.296260000	-2.418580000
1	2.800319000	-1.263564000	1.553853000
1	5.096338000	-0.829046000	2.415922000
1	6.949290000	-0.421088000	0.801992000
1	6.400668000	0.138143000	-1.562295000
1	4.692778000	2.002394000	-1.666027000
1	6.363178000	1.938330000	0.230407000
1	5.825863000	1.539233000	1.866795000
1	3.385898000	1.036163000	2.306213000
1	2.825551000	-3.054889000	-0.234947000
1	3.362923000	-2.658294000	-1.871871000
1	4.512495000	-3.136529000	1.671168000
1	6.217725000	-2.793504000	1.358321000

1	5.820112000	-2.165932000	-2.320151000
1	6.988884000	-2.221338000	-0.995656000
1	5.155111000	-3.875279000	-0.625864000
1	-6.534144000	-0.015702000	1.270623000
1	-4.834828000	-1.836796000	1.735512000
1	-6.035727000	2.362571000	1.831475000
1	-6.321372000	-1.993412000	-0.307178000
1	-7.071796000	2.262850000	0.403201000
6	-5.786971000	0.538748000	0.685473000
6	-6.065271000	2.043700000	0.781787000
1	-3.134127000	-3.665061000	2.207532000
1	-4.630615000	-3.808896000	0.154358000
1	-4.332120000	0.535704000	2.291092000
6	-4.081042000	-1.285007000	1.151076000
1	-6.854778000	0.284403000	-1.181343000
6	-5.566640000	-1.429808000	-0.873523000
6	-4.385404000	0.219069000	1.236999000
6	-5.853099000	0.071700000	-0.782383000
1	-2.633148000	-1.284056000	2.756527000
6	-2.400395000	-3.109142000	1.610023000
6	-3.870769000	-3.250880000	-0.410453000
6	-2.680567000	-1.604914000	1.706367000
6	-4.173466000	-1.750046000	-0.323013000
1	-5.630963000	-1.764091000	-1.918580000
6	-5.017667000	2.816694000	-0.032387000
1	-1.408163000	-3.331708000	2.022880000
6	-2.471529000	-3.554661000	0.142305000
1	-3.943413000	-3.575874000	-1.457757000
1	-5.215774000	3.892570000	0.036757000
1	-2.272515000	-4.630293000	0.072195000
1	-3.548720000	2.837857000	1.570379000
6	-3.320557000	1.010023000	0.438223000
1	-6.079723000	2.594197000	-1.913649000
6	-4.809925000	0.865316000	-1.594410000
6	-3.620094000	2.511437000	0.523433000
6	-5.088311000	2.370038000	-1.499783000
1	-1.861180000	1.022004000	2.035833000
6	-1.639146000	-0.810567000	0.892789000
6	-3.110254000	-0.958803000	-1.123073000
6	-1.927630000	0.689686000	0.989673000
6	-3.411328000	0.545112000	-1.036382000
1	-4.855019000	0.544015000	-2.644562000
6	-1.425826000	-2.780037000	-0.673110000
1	-0.635673000	-1.025272000	1.290454000
6	-1.707889000	-1.276261000	-0.575424000
1	-3.165181000	-1.274774000	-2.177300000
1	-2.856973000	3.066538000	-0.040552000
1	-4.353108000	2.924033000	-2.097271000
1	-0.417597000	-2.999102000	-0.296223000
1	-1.174336000	1.256869000	0.425236000

1	-1.455184000	-3.098048000	-1.723075000
1	-2.654445000	1.095560000	-1.618893000
1	-0.965619000	-0.718711000	-1.164233000

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**D4**

6	4.251409000	-1.602644000	1.196508000
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6	4.500429000	-3.008439000	0.636702000
6	3.762012000	-2.235751000	-1.626600000
6	2.089078000	-3.174816000	-0.021332000
6	3.535455000	-3.280984000	-0.526196000
6	2.551210000	-0.072780000	2.261872000
6	4.224637000	0.874477000	0.639002000
6	2.775709000	0.982905000	1.174769000
6	1.823147000	0.705630000	-0.012611000
6	2.040939000	1.763530000	-1.109701000
6	3.488934000	1.640382000	-1.625222000
6	4.450232000	1.933551000	-0.455538000
6	4.469746000	-0.543892000	0.100308000
6	3.737361000	0.233721000	-2.176062000
6	2.066868000	-0.712318000	-0.550428000
6	3.515660000	-0.821384000	-1.088018000
6	2.524294000	2.397212000	1.711206000
6	1.790763000	3.169995000	-0.552904000
6	4.200073000	3.338172000	0.106072000
6	2.753838000	3.442425000	0.611201000
1	4.945074000	-1.404115000	2.025648000
1	2.641005000	-2.223479000	2.504365000
1	0.809132000	-1.692318000	0.910728000
1	5.538362000	-3.094578000	0.290739000
1	4.357665000	-3.756413000	1.426974000
1	3.088152000	-2.424884000	-2.473873000
1	4.789786000	-2.304874000	-2.009502000
1	1.390679000	-3.372257000	-0.846201000
1	1.900455000	-3.930342000	0.752471000
1	3.714390000	-4.285029000	-0.927901000
1	1.519663000	0.005040000	2.635802000
1	3.219643000	0.128430000	3.110777000
1	4.917838000	1.065269000	1.474046000
1	0.787591000	0.775474000	0.358996000
1	1.347996000	1.561709000	-1.940494000
1	3.651341000	2.384519000	-2.417418000
1	5.485381000	1.856156000	-0.816842000
1	5.506388000	-0.613289000	-0.266780000
1	4.764975000	0.153193000	-2.557557000
1	3.062720000	0.034093000	-3.020467000
1	1.371459000	-0.903406000	-1.386160000
1	1.492516000	2.463422000	2.086360000
1	3.191691000	2.588823000	2.563007000

1	0.752138000	3.258146000	-0.208844000
1	1.935440000	3.916653000	-1.344202000
1	4.900618000	3.542544000	0.925789000
1	4.381033000	4.090478000	-0.672163000
1	2.573601000	4.446372000	1.012645000
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1	-4.900660000	-3.542517000	-0.925818000
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1	-4.381034000	-4.090488000	0.672108000
6	-4.450229000	-1.933555000	0.455533000
6	-4.200091000	-3.338166000	-0.106116000
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1	-4.789712000	2.304838000	2.009603000
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1	-3.651287000	-2.384572000	2.417380000
6	-3.737301000	-0.233767000	2.176075000
6	-4.224659000	-0.874458000	-0.638990000
6	-3.488898000	-1.640418000	1.625197000
1	-4.945124000	1.404171000	-2.025563000
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6	-3.761950000	2.235717000	1.626669000
6	-4.251434000	1.602676000	-1.196438000
6	-3.515624000	0.821360000	1.088048000
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6	-1.790763000	-3.170014000	0.552798000
1	-3.219733000	-0.128362000	-3.110776000
6	-2.804187000	1.479453000	-1.712199000
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6	-2.551274000	0.072826000	-2.261886000
6	-1.823149000	-0.705638000	0.012561000
1	-1.347951000	-1.561761000	1.940412000
6	-2.089055000	3.174807000	0.021373000
1	-2.641063000	2.223531000	-2.504328000
6	-1.842698000	1.771427000	-0.543823000
1	-1.371414000	0.903364000	1.386131000
1	-1.492587000	-2.463385000	-2.086461000
1	-0.752148000	-3.258159000	0.208707000

1	-1.900452000	3.930349000	-0.752419000
1	-1.519738000	-0.004991000	-2.635848000
1	-1.390629000	3.372226000	0.846225000
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**D5**

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6	-5.142666000	2.470038000	-1.367393000
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6	-4.069098000	3.094167000	0.806200000
6	-3.933872000	3.162996000	-0.721698000
6	-5.379948000	-0.549768000	1.058804000
6	-3.946123000	-1.204154000	-0.900156000
6	-4.103129000	-1.284314000	0.638064000
6	-2.874527000	-0.580604000	1.264932000
6	-1.588689000	-1.314687000	0.844273000
6	-1.455616000	-1.226766000	-0.689335000
6	-2.663533000	-1.940779000	-1.326973000
6	-3.914309000	0.268488000	-1.339271000
6	-1.407664000	0.237659000	-1.130395000
6	-2.842708000	0.891334000	0.826176000
6	-2.685036000	0.971365000	-0.712078000
6	-4.132588000	-2.753331000	1.077940000
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6	-2.713538000	-3.406062000	-0.878370000
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1	-6.255679000	1.426999000	0.924061000
1	-4.216695000	1.576735000	2.347493000
1	-5.066368000	2.522601000	-2.460934000
1	-6.068254000	2.985279000	-1.080580000
1	-1.771010000	2.929442000	-0.703121000
1	-2.529343000	2.493044000	-2.240191000
1	-3.217796000	3.597507000	1.281909000
1	-4.978388000	3.618305000	1.126981000
1	-3.893083000	4.210333000	-1.042561000
1	-5.492473000	-0.610134000	2.150449000
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1	-4.816401000	-1.697003000	-1.362656000
1	-2.972689000	-0.625772000	2.361510000
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1	-0.534600000	-1.739577000	-1.003317000
1	-2.571240000	-1.889423000	-2.420959000
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1	-0.539636000	0.738350000	-0.677825000
1	-1.971285000	1.383993000	1.288322000

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1	-3.562756000	-3.914003000	-1.352878000
1	-1.801441000	-3.925857000	-1.199542000
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1	4.971466000	1.498865000	2.290865000
1	5.224505000	-0.853645000	1.376868000
1	5.430631000	3.481257000	0.847811000
1	3.399650000	-0.342405000	3.062497000
1	4.157469000	3.842833000	2.018899000
6	4.284492000	1.748748000	1.470075000
6	4.398776000	3.240580000	1.133763000
1	5.475673000	-3.210492000	0.467849000
1	3.640098000	-2.684825000	2.159434000
1	5.679334000	1.121777000	-0.065438000
6	4.535953000	-0.607448000	0.552541000
1	2.583232000	2.001076000	2.785920000
6	2.731835000	-0.086692000	2.227811000
6	4.645670000	0.893927000	0.240840000
6	2.844416000	1.404526000	1.900708000
1	5.926224000	-1.230858000	-0.981452000
6	4.777775000	-2.953719000	-0.339254000
6	2.976449000	-2.434368000	1.320045000
6	4.895876000	-1.462627000	-0.676911000
6	3.093451000	-0.938015000	1.007037000
1	1.707743000	-0.327296000	2.548232000
6	3.441034000	3.586660000	-0.015604000
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1	1.948551000	-2.656617000	1.642239000
1	3.523516000	4.652644000	-0.257302000
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1	4.832159000	2.979116000	-1.571688000
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1	1.721149000	3.866701000	1.281337000
6	1.889312000	1.771170000	0.747408000
6	3.808105000	2.747535000	-1.246972000
6	2.001195000	3.261977000	0.409415000
1	5.080241000	0.634045000	-2.478327000
6	3.939100000	-1.093666000	-1.828900000
6	2.148714000	-0.580550000	-0.165129000
6	4.056702000	0.398067000	-2.154699000
6	2.258506000	0.918362000	-0.479710000
1	0.857565000	1.532957000	1.049817000
6	2.380068000	-2.926801000	-1.059327000
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1	1.117920000	-0.806188000	0.147869000

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1	3.386965000	0.657152000	-2.986719000
1	1.347165000	-3.164826000	-0.769568000
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**D6**

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6	1.678206000	1.311182000	0.373451000
6	2.653393000	2.956967000	-1.238294000
6	2.041268000	2.786249000	0.159317000
6	6.205525000	1.625004000	-0.425834000
6	5.218723000	-0.034973000	1.184556000
6	5.856591000	0.148402000	-0.214551000
6	4.803256000	-0.287560000	-1.262670000
6	4.449409000	-1.771292000	-1.053780000
6	3.820543000	-1.930988000	0.344773000
6	4.865892000	-1.518228000	1.400324000
6	3.973564000	0.857648000	1.304598000
6	2.570536000	-1.055036000	0.469413000
6	3.557675000	0.604152000	-1.142822000
6	2.920576000	0.421391000	0.256824000
6	7.100768000	-0.739868000	-0.334400000
6	5.706863000	-2.640022000	-1.178370000
6	6.123446000	-2.386954000	1.276983000
6	6.735496000	-2.214963000	-0.120688000
1	5.062410000	2.642593000	1.852908000
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1	2.639443000	3.105771000	2.222432000
1	3.330660000	4.268454000	1.084974000
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1	1.218938000	1.173435000	1.363415000
1	1.923593000	2.668773000	-2.005618000
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1	1.139841000	3.404119000	0.247486000
1	6.661722000	1.753588000	-1.417473000
1	6.955413000	1.932056000	0.316740000
1	5.955607000	0.274170000	1.943272000
1	5.240402000	-0.158796000	-2.265933000
1	3.713118000	-2.071097000	-1.812773000
1	3.552545000	-2.985495000	0.499038000
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1	2.118126000	-1.183719000	1.463371000

1	1.815253000	-1.362720000	-0.269641000
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1	5.868752000	-3.440521000	1.448759000
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6	-2.408228000	-0.118714000	1.178064000
6	-1.297735000	-1.175656000	1.155853000
1	-7.316143000	1.250526000	2.200858000
1	-5.826787000	2.835491000	0.878259000
1	-3.861102000	-1.420294000	2.121687000
6	-4.920997000	0.244955000	1.237882000
1	-1.354818000	1.266736000	-0.108483000
6	-3.448290000	1.815479000	-0.060560000
6	-3.790294000	-0.795972000	1.216437000
6	-2.333066000	0.766590000	-0.081561000
1	-6.364550000	-1.054349000	2.187005000
6	-7.413174000	0.625209000	1.304202000
6	-5.950537000	2.183804000	0.002048000
6	-6.302909000	-0.432320000	1.282921000
6	-4.824003000	1.143510000	-0.019432000
1	-3.381680000	2.455779000	-0.951422000
6	-1.454353000	-2.066278000	-0.084524000
1	-8.394493000	0.136231000	1.353016000
6	-7.321706000	1.496122000	0.043016000
1	-5.872936000	2.822257000	-0.889061000
1	-0.659314000	-2.821671000	-0.098838000
1	-8.114550000	2.252936000	0.057845000
1	-2.902359000	-3.392670000	0.848625000
6	-3.952388000	-1.713772000	-0.020399000
1	-0.381580000	-0.708245000	-1.397618000
6	-2.473597000	-0.136995000	-1.322933000
6	-2.825579000	-2.754537000	-0.042768000
6	-1.364568000	-1.195879000	-1.346044000
1	-5.395147000	-3.025684000	0.911849000
6	-6.443904000	-1.336332000	0.042087000
6	-4.986154000	0.225778000	-1.256077000
6	-5.328632000	-2.385578000	0.020870000
6	-3.855468000	-0.814978000	-1.277674000
1	-2.412515000	0.485318000	-2.226895000
6	-7.478242000	0.605894000	-1.198219000
1	-7.423001000	-1.834637000	0.071393000

6	-6.368137000	-0.451747000	-1.218168000
1	-4.915379000	0.850023000	-2.161378000
1	-2.950471000	-3.406334000	-0.918755000
1	-1.463638000	-1.820953000	-2.242760000
1	-8.460745000	0.116957000	-1.188658000
1	-5.441698000	-3.039118000	-0.855571000
1	-7.427814000	1.217376000	-2.108144000
1	-3.973256000	-1.453012000	-2.168374000
1	-6.476614000	-1.087689000	-2.108066000

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6	-4.453950000	-2.156395000	0.127255000
6	-3.991657000	-1.860829000	-1.313735000
6	-2.450014000	-1.830588000	-1.334818000
6	-3.884746000	-3.497127000	0.607122000
6	-1.866034000	-2.319391000	1.500078000
6	-1.879752000	-3.170818000	-0.855589000
6	-2.349954000	-3.448003000	0.579770000
6	-4.555487000	-0.517760000	-1.786397000
6	-4.527326000	0.343279000	0.576764000
6	-4.077591000	0.620557000	-0.879499000
6	-2.530063000	0.664954000	-0.881523000
6	-2.045710000	1.805947000	0.029609000
6	-2.505942000	1.513288000	1.470775000
6	-4.047414000	1.485388000	1.491954000
6	-3.971504000	-1.013258000	1.039489000
6	-1.944818000	0.169949000	1.945030000
6	-1.975197000	-0.689715000	-0.417517000
6	-2.423578000	-0.967706000	1.037764000
6	-4.631407000	1.973514000	-1.342520000
6	-2.606715000	3.148107000	-0.452412000
6	-4.613448000	2.826761000	1.010229000
6	-4.141705000	3.102424000	-0.425022000
1	-5.552366000	-2.189452000	0.149877000
1	-4.343489000	-2.665305000	-1.974660000
1	-2.108803000	-1.626538000	-2.359898000
1	-4.235763000	-3.708999000	1.625109000
1	-4.246291000	-4.308613000	-0.037274000
1	-0.766868000	-2.277904000	1.507209000
1	-2.186735000	-2.510158000	2.533828000
1	-0.782199000	-3.147114000	-0.896030000
1	-2.210898000	-3.977834000	-1.521641000
1	-1.942682000	-4.405687000	0.923986000
1	-4.238709000	-0.317783000	-2.819671000
1	-5.654184000	-0.548055000	-1.785612000
1	-5.628411000	0.304575000	0.596288000
1	-2.187726000	0.857397000	-1.911915000
1	-0.947633000	1.833104000	0.005936000
1	-2.151331000	2.318480000	2.129900000
1	-4.387623000	1.285177000	2.517753000

1	-4.311055000	-1.206595000	2.069827000
1	-2.263540000	-0.028953000	2.977989000
1	-0.844773000	0.197283000	1.947707000
1	-0.874886000	-0.647228000	-0.435065000
1	-4.313349000	2.161178000	-2.377566000
1	-5.729751000	1.936225000	-1.343827000
1	-2.253112000	3.356321000	-1.470652000
1	-2.241655000	3.959226000	0.191061000
1	-5.710060000	2.804375000	1.047130000
1	-4.281698000	3.633286000	1.676436000
1	-4.547022000	4.060672000	-0.770002000
1	4.387656000	-1.285117000	-2.517772000
1	4.311088000	1.206643000	-2.069785000
1	5.710070000	-2.804354000	-1.047170000
1	2.263575000	0.029025000	-2.978007000
1	4.281716000	-3.633247000	-1.676516000
6	4.047432000	-1.485353000	-1.491983000
6	4.613457000	-2.826739000	-1.010285000
1	4.235792000	3.709038000	-1.625004000
1	2.186784000	2.510221000	-2.533787000
1	5.628418000	-0.304566000	-0.596264000
6	3.971520000	1.013282000	-1.039457000
1	2.151357000	-2.318427000	-2.129977000
6	1.944843000	-0.169901000	-1.945056000
6	4.527332000	-0.343268000	-0.576758000
6	2.505959000	-1.513252000	-1.470828000
1	5.552369000	2.189450000	-0.149790000
6	3.884759000	3.497140000	-0.607029000
6	1.866062000	2.319429000	-1.500048000
6	4.453953000	2.156395000	-0.127187000
6	2.423594000	0.967731000	-1.037757000
1	0.844797000	-0.197234000	-1.947742000
6	4.141695000	-3.102438000	0.424954000
1	4.246294000	4.308609000	0.037395000
6	2.349966000	3.448016000	-0.579702000
1	0.766896000	2.277945000	-1.507204000
1	4.547006000	-4.060694000	0.769915000
1	1.942700000	4.405710000	-0.923901000
1	5.729728000	-1.936263000	1.343810000
6	4.077576000	-0.620582000	0.879492000
1	2.241653000	-3.959223000	-0.191177000
6	2.045707000	-1.805947000	-0.029675000
6	4.631384000	-1.973551000	1.342487000
6	2.606704000	-3.148119000	0.452320000
1	5.654156000	0.548006000	1.785657000
6	3.991637000	1.860793000	1.313789000
6	1.975191000	0.689704000	0.417510000
6	4.555459000	0.517712000	1.786426000
6	2.530048000	-0.664977000	0.881492000
1	0.947629000	-1.833105000	-0.006016000

6	1.879740000	3.170795000	0.855642000
1	4.343460000	2.665252000	1.974740000
6	2.449994000	1.830554000	1.334846000
1	0.874880000	0.647219000	0.435038000
1	4.313311000	-2.161241000	2.377523000
1	2.253086000	-3.356358000	1.470551000
1	2.210874000	3.977795000	1.521719000
1	4.238665000	0.317709000	2.819690000
1	0.782186000	3.147089000	0.896063000
1	2.187695000	-0.857444000	1.911873000
1	2.108766000	1.626478000	2.359917000

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6	4.996353000	-1.318705000	-0.202756000
6	4.554741000	-1.198613000	1.269368000
6	3.083458000	-1.646876000	1.375537000
6	4.838642000	-2.762994000	-0.694193000
6	2.503599000	-2.255901000	-1.435901000
6	2.927123000	-3.091560000	0.887474000
6	3.368177000	-3.191214000	-0.579849000
6	4.704149000	0.246819000	1.752696000
6	4.268116000	1.086704000	-0.576497000
6	3.843118000	1.192006000	0.908993000
6	2.360458000	0.755301000	0.996147000
6	1.492916000	1.700082000	0.147368000
6	1.935929000	1.585922000	-1.325176000
6	3.406427000	2.037069000	-1.428587000
6	4.129920000	-0.369522000	-1.050111000
6	1.794963000	0.143309000	-1.816131000
6	2.221066000	-0.698810000	0.522327000
6	2.646135000	-0.804365000	-0.963677000
6	3.977889000	2.643920000	1.384387000
6	1.639891000	3.144761000	0.638130000
6	3.558637000	3.481079000	-0.935893000
6	3.109821000	3.577554000	0.529304000
1	6.048017000	-1.010327000	-0.286637000
1	5.176714000	-1.863054000	1.885359000
1	2.761277000	-1.571504000	2.423729000
1	5.173299000	-2.840943000	-1.736493000
1	5.471971000	-3.432175000	-0.097975000
1	1.446115000	-2.553325000	-1.376798000
1	2.799440000	-2.326982000	-2.491950000
1	1.881640000	-3.409582000	0.990502000
1	3.533507000	-3.763916000	1.507823000
1	3.255370000	-4.223379000	-0.931177000
1	4.405004000	0.324856000	2.807438000
1	5.756114000	0.559365000	1.691366000
1	5.324506000	1.390248000	-0.655647000
1	2.040413000	0.821071000	2.048774000
1	0.444651000	1.382379000	0.231271000

1	1.311835000	2.251368000	-1.939179000
1	3.729147000	1.965977000	-2.476815000
1	4.447853000	-0.434966000	-2.103142000
1	2.111766000	0.069526000	-2.866013000
1	0.741319000	-0.168860000	-1.779115000
1	1.164002000	-1.003369000	0.604650000
1	3.679398000	2.709559000	2.440042000
1	5.032018000	2.949421000	1.327299000
1	1.299762000	3.222003000	1.679087000
1	1.004558000	3.809430000	0.037870000
1	4.604552000	3.799937000	-1.029870000
1	2.955791000	4.154011000	-1.558890000
1	3.219076000	4.609495000	0.882521000
1	-5.386161000	0.919775000	-1.857004000
1	-4.967006000	-1.492171000	-1.201309000
1	-6.073657000	2.604550000	-0.151182000
1	-3.558637000	-0.419961000	-3.014601000
1	-5.092053000	3.358478000	-1.412520000
6	-4.664681000	1.255762000	-1.098933000
6	-5.064572000	2.642825000	-0.580969000
1	-4.549961000	-3.911346000	-0.548759000
1	-3.136776000	-2.818052000	-2.366931000
1	-5.650419000	0.184594000	0.506148000
6	-4.244402000	-1.160919000	-0.438239000
1	-3.266719000	2.018938000	-2.565731000
6	-2.856856000	-0.082684000	-2.238917000
6	-4.645889000	0.238071000	0.056406000
6	-3.259455000	1.304166000	-1.731045000
1	-5.231925000	-2.228345000	1.161650000
6	-3.823494000	-3.564916000	0.197360000
6	-2.435602000	-2.489840000	-1.587012000
6	-4.228194000	-2.179748000	0.716428000
6	-2.841843000	-1.097009000	-1.091222000
1	-1.859947000	-0.040658000	-2.700966000
6	-4.058517000	3.109018000	0.481492000
1	-3.831846000	-4.290103000	1.021014000
6	-2.422529000	-3.494506000	-0.427347000
1	-1.439851000	-2.432885000	-2.050422000
1	-4.345525000	4.099555000	0.852980000
1	-2.132477000	-4.484156000	-0.798752000
1	-5.043870000	2.054922000	2.107513000
6	-3.651247000	0.709497000	1.145681000
1	-2.644663000	3.902960000	-0.964268000
6	-2.259569000	1.789709000	-0.663428000
6	-4.049776000	2.104506000	1.641628000
6	-2.656647000	3.175555000	-0.142567000
1	-4.628604000	-0.347611000	2.757807000
6	-3.230117000	-1.692421000	1.786363000
6	-1.849444000	-0.625861000	-0.000678000
6	-3.633208000	-0.304945000	2.293729000

6	-2.248745000	0.772238000	0.492396000
1	-1.255725000	1.833133000	-1.112535000
6	-1.417868000	-3.024655000	0.634059000
1	-3.223339000	-2.406961000	2.621279000
6	-1.824678000	-1.641337000	1.154546000
1	-0.845207000	-0.572500000	-0.450479000
1	-3.344223000	2.428846000	2.419257000
1	-1.926578000	3.514944000	0.604160000
1	-1.378825000	-3.742708000	1.463245000
1	-2.930130000	0.033355000	3.067794000
1	-0.410628000	-2.974758000	0.198210000
1	-1.527741000	1.102073000	1.259252000
1	-1.101795000	-1.301010000	1.911003000

**Table S7.** Geometries of [121]tetramantane tetramers in Cartesian coordinates in Å computed at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.

<b>Type A (+5°) on Au(111)</b>			
6	3.866366000	4.406186000	1.577867000
6	4.229921000	3.106913000	0.825813000
6	4.320585000	3.425656000	-0.682845000
6	4.924137000	5.489974000	1.321965000
6	3.626909000	6.282126000	-0.672517000
6	5.378892000	4.508285000	-0.941417000
6	5.000314000	5.793102000	-0.184472000
6	3.167781000	2.030958000	1.079080000
6	1.405020000	3.812286000	1.336586000
6	1.789726000	2.502921000	0.597500000
6	1.857819000	2.834821000	-0.917058000
6	0.474575000	3.310246000	-1.405524000
6	0.111020000	4.609519000	-0.653471000
6	0.020357000	4.290776000	0.855188000
6	2.483122000	4.881611000	1.089401000
6	1.173160000	5.685474000	-0.906737000
6	2.935921000	3.904146000	-1.164243000
6	2.551215000	5.213511000	-0.425157000
6	0.714032000	1.434306000	0.844860000
6	-0.583196000	2.226458000	-1.149622000
6	-1.037951000	3.208147000	1.113760000
6	-0.659373000	1.923330000	0.356815000
1	3.808722000	4.192130000	2.653882000
1	5.208036000	2.750987000	1.176709000
1	4.588325000	2.509188000	-1.226311000
1	4.668119000	6.401439000	1.877210000
1	5.902250000	5.153730000	1.689055000
1	3.667803000	6.518146000	-1.744466000
1	3.347966000	7.208584000	-0.152594000
1	5.450632000	4.712216000	-2.017464000
1	6.365095000	4.154578000	-0.614590000

1	5.754853000	6.567425000	-0.368716000
1	3.439536000	1.102562000	0.558543000
1	3.119696000	1.793006000	2.150432000
1	1.355712000	3.599564000	2.414903000
1	2.134289000	1.918836000	-1.460185000
1	0.532219000	3.524302000	-2.481539000
1	-0.867095000	4.965445000	-1.004366000
1	-0.247383000	5.207244000	1.398654000
1	2.206652000	5.797596000	1.632528000
1	0.901406000	6.613870000	-0.386200000
1	1.221246000	5.923426000	-1.978090000
1	2.985229000	4.116868000	-2.242560000
1	0.992975000	0.507848000	0.324937000
1	0.673139000	1.198286000	1.916809000
1	-0.327178000	1.314993000	-1.704867000
1	-1.561309000	2.562702000	-1.516712000
1	-1.109690000	3.004216000	2.189807000
1	-2.024154000	3.561854000	0.786933000
1	-1.413912000	1.149007000	0.541059000
6	-5.936119000	1.973196000	1.535026000
6	-5.572565000	0.673923000	0.782972000
6	-5.481901000	0.992666000	-0.725687000
6	-4.878349000	3.056984000	1.279124000
6	-6.175577000	3.849136000	-0.715358000
6	-4.423594000	2.075296000	-0.984258000
6	-4.802172000	3.360112000	-0.227313000
6	-6.634705000	-0.402032000	1.036239000
6	-8.397463000	1.379297000	1.293745000
6	-8.012762000	0.069930000	0.554659000
6	-7.944664000	0.401832000	-0.959900000
6	-9.327913000	0.877255000	-1.448365000
6	-9.691464000	2.176530000	-0.696312000
6	-9.782132000	1.857786000	0.812347000
6	-7.319363000	2.448621000	1.046560000
6	-8.629329000	3.252483000	-0.949578000
6	-6.866565000	1.471156000	-1.207084000
6	-7.251271000	2.780521000	-0.467999000
6	-9.088450000	-0.998683000	0.802019000
6	-10.385683000	-0.206533000	-1.192463000
6	-10.840438000	0.775156000	1.070919000
6	-10.461857000	-0.509659000	0.313974000
1	-5.993763000	1.759141000	2.611040000
1	-4.594449000	0.317997000	1.133868000
1	-5.214161000	0.076198000	-1.269152000
1	-5.134366000	3.968449000	1.834369000
1	-3.900236000	2.720740000	1.646214000
1	-6.134683000	4.085156000	-1.787308000
1	-6.454519000	4.775594000	-0.195435000
1	-4.351854000	2.279226000	-2.060305000
1	-3.437391000	1.721588000	-0.657431000

1	-4.047633000	4.134435000	-0.411557000
1	-6.362950000	-1.330428000	0.515702000
1	-6.682790000	-0.639984000	2.107591000
1	-8.446776000	1.166573000	2.372061000
1	-7.668194000	-0.514153000	-1.503026000
1	-9.270265000	1.091312000	-2.524380000
1	-10.669577000	2.532456000	-1.047208000
1	-10.049872000	2.774253000	1.355812000
1	-7.595833000	3.364606000	1.589686000
1	-8.901084000	4.180879000	-0.429041000
1	-8.581239000	3.490436000	-2.020931000
1	-6.817257000	1.683878000	-2.285401000
1	-8.809513000	-1.925142000	0.282095000
1	-9.129346000	-1.234704000	1.873968000
1	-10.129664000	-1.117997000	-1.747708000
1	-11.363796000	0.129712000	-1.559554000
1	-10.912171000	0.571227000	2.146966000
1	-11.826637000	1.128865000	0.744092000
1	-11.216398000	-1.283983000	0.498217000
6	9.327911000	-0.877255000	1.448365000
6	9.691465000	-2.176530000	0.696312000
6	9.782130000	-1.857786000	-0.812347000
6	10.385681000	0.206532000	1.192463000
6	9.088453000	0.998683000	-0.802019000
6	10.840436000	-0.775157000	-1.070919000
6	10.461858000	0.509660000	-0.313974000
6	8.629325000	-3.252485000	0.949578000
6	6.866565000	-1.471156000	1.207084000
6	7.251270000	-2.780521000	0.467999000
6	7.319363000	-2.448621000	-1.046560000
6	5.936120000	-1.973197000	-1.535026000
6	5.572564000	-0.673922000	-0.782972000
6	5.481901000	-0.992666000	0.725687000
6	7.944667000	-0.401831000	0.959900000
6	6.634704000	0.402032000	-1.036239000
6	8.397465000	-1.379296000	-1.293745000
6	8.012760000	-0.069931000	-0.554659000
6	6.175577000	-3.849135000	0.715358000
6	4.878349000	-3.056984000	-1.279124000
6	4.423594000	-2.075295000	0.984258000
6	4.802172000	-3.360112000	0.227313000
1	9.270266000	-1.091312000	2.524380000
1	10.669581000	-2.532455000	1.047208000
1	10.049869000	-2.774254000	-1.355812000
1	10.129664000	1.117997000	1.747708000
1	11.363794000	-0.129712000	1.559554000
1	9.129347000	1.234704000	-1.873968000
1	8.809511000	1.925141000	-0.282095000
1	10.912176000	-0.571226000	-2.146966000
1	11.826639000	-1.128864000	-0.744092000

1	11.216398000	1.283983000	-0.498217000
1	8.901080000	-4.180880000	0.429041000
1	8.581241000	-3.490436000	2.020931000
1	6.817256000	-1.683878000	2.285401000
1	7.595834000	-3.364606000	-1.589686000
1	5.993764000	-1.759140000	-2.611040000
1	4.594450000	-0.317997000	-1.133868000
1	5.214162000	-0.076198000	1.269152000
1	7.668197000	0.514154000	1.503026000
1	6.362950000	1.330428000	-0.515702000
1	6.682790000	0.639984000	-2.107591000
1	8.446773000	-1.166574000	-2.372061000
1	6.454520000	-4.775593000	0.195435000
1	6.134683000	-4.085157000	1.787308000
1	5.134366000	-3.968449000	-1.834369000
1	3.900236000	-2.720740000	-1.646214000
1	4.351854000	-2.279226000	2.060305000
1	3.437391000	-1.721588000	0.657431000
1	4.047632000	-4.134435000	0.411557000
6	-0.474575000	-3.310245000	1.405524000
6	-0.111021000	-4.609520000	0.653471000
6	-0.020356000	-4.290776000	-0.855188000
6	0.583195000	-2.226458000	1.149622000
6	-0.714032000	-1.434307000	-0.844860000
6	1.037951000	-3.208147000	-1.113760000
6	0.659372000	-1.923330000	-0.356815000
6	-1.173160000	-5.685475000	0.906737000
6	-2.935920000	-3.904146000	1.164243000
6	-2.551215000	-5.213511000	0.425157000
6	-2.483123000	-4.881611000	-1.089401000
6	-3.866366000	-4.406186000	-1.577867000
6	-4.229921000	-3.106912000	-0.825813000
6	-4.320585000	-3.425656000	0.682845000
6	-1.857818000	-2.834821000	0.917058000
6	-3.167781000	-2.030958000	-1.079080000
6	-1.405020000	-3.812286000	-1.336586000
6	-1.789726000	-2.502921000	-0.597500000
6	-3.626908000	-6.282125000	0.672517000
6	-4.924137000	-5.489974000	-1.321965000
6	-5.378891000	-4.508285000	0.941417000
6	-5.000314000	-5.793102000	0.184472000
1	-0.532219000	-3.524302000	2.481539000
1	0.867095000	-4.965445000	1.004366000
1	0.247383000	-5.207244000	-1.398654000
1	0.327179000	-1.314993000	1.704867000
1	1.561308000	-2.562702000	1.516712000
1	-0.673139000	-1.198286000	-1.916809000
1	-0.992975000	-0.507849000	-0.324937000
1	1.109690000	-3.004216000	-2.189807000
1	2.024153000	-3.561854000	-0.786933000

1	1.413913000	-1.149007000	-0.541059000
1	-0.901406000	-6.613870000	0.386200000
1	-1.221245000	-5.923426000	1.978090000
1	-2.985229000	-4.116868000	2.242560000
1	-2.206652000	-5.797596000	-1.632528000
1	-3.808722000	-4.192130000	-2.653882000
1	-5.208036000	-2.750987000	-1.176709000
1	-4.588324000	-2.509188000	1.226311000
1	-2.134289000	-1.918836000	1.460185000
1	-3.439536000	-1.102562000	-0.558543000
1	-3.119696000	-1.793006000	-2.150432000
1	-1.355713000	-3.599564000	-2.414903000
1	-3.347966000	-7.208583000	0.152594000
1	-3.667803000	-6.518147000	1.744466000
1	-4.668120000	-6.401439000	-1.877210000
1	-5.902248000	-5.153730000	-1.689055000
1	-5.450631000	-4.712216000	2.017464000
1	-6.365099000	-4.154579000	0.614590000
1	-5.754850000	-6.567424000	0.368716000

#### Type A (-5°) on Au(111)

6	-0.372654000	3.334412000	-0.988409000
6	-0.094723000	4.640260000	-0.211633000
6	-0.240452000	4.349967000	1.298454000
6	0.607390000	2.233100000	-0.557615000
6	-0.994862000	1.509724000	1.230619000
6	0.739749000	3.249855000	1.731950000
6	0.448064000	1.958687000	0.947827000
6	-1.079676000	5.733891000	-0.640355000
6	-2.826840000	3.986740000	-1.131929000
6	-2.525801000	5.301952000	-0.364939000
6	-2.695051000	4.999120000	1.147784000
6	-4.147428000	4.563973000	1.429278000
6	-4.425360000	3.258125000	0.652501000
6	-4.279631000	3.548418000	-0.857586000
6	-1.825032000	2.899265000	-0.706916000
6	-3.440407000	2.164494000	1.081223000
6	-1.693242000	3.911645000	1.572798000
6	-1.994282000	2.596433000	0.805807000
6	-3.525221000	6.388661000	-0.789751000
6	-5.127473000	5.665285000	0.998483000
6	-5.259832000	4.648530000	-1.291082000
6	-4.968147000	5.939698000	-0.506959000
1	-0.262107000	3.528029000	-2.064163000
1	0.933593000	4.967586000	-0.416438000
1	-0.035199000	5.271085000	1.860916000
1	0.415622000	1.316489000	-1.130030000
1	1.637660000	2.540428000	-0.778101000
1	-1.121893000	1.294436000	2.300183000
1	-1.214982000	0.579337000	0.689896000

1	0.643375000	3.066050000	2.809697000
1	1.772373000	3.575269000	1.552193000
1	1.146872000	1.171899000	1.256828000
1	-0.866704000	6.666384000	-0.100144000
1	-0.959795000	5.951277000	-1.710448000
1	-2.707740000	4.178795000	-2.208675000
1	-2.481131000	5.919558000	1.711239000
1	-4.257976000	4.370356000	2.505031000
1	-5.453676000	2.930799000	0.857307000
1	-4.484884000	2.627300000	-1.420047000
1	-2.038952000	1.978827000	-1.270371000
1	-3.653379000	1.232001000	0.541013000
1	-3.560288000	1.947108000	2.151316000
1	-1.812343000	3.719590000	2.649544000
1	-3.305100000	7.319048000	-0.249028000
1	-3.398190000	6.603949000	-1.859315000
1	-4.935705000	6.581896000	1.570898000
1	-6.157743000	5.357957000	1.218969000
1	-5.163458000	4.832334000	-2.368828000
1	-6.292456000	4.323116000	-1.111324000
1	-5.666955000	6.726486000	-0.815960000
6	9.426316000	0.900385000	-1.244586000
6	9.704252000	2.206232000	-0.467810000
6	9.558522000	1.915939000	1.042277000
6	10.406364000	-0.200928000	-0.813791000
6	8.804108000	-0.924302000	0.974442000
6	10.538722000	0.815827000	1.475773000
6	10.247038000	-0.475340000	0.691650000
6	8.719299000	3.299863000	-0.896531000
6	6.972133000	1.552713000	-1.388106000
6	7.273172000	2.867925000	-0.621115000
6	7.103922000	2.565092000	0.891607000
6	5.651545000	2.129945000	1.173101000
6	5.373613000	0.824097000	0.396324000
6	5.519342000	1.114391000	-1.113762000
6	7.973941000	0.465238000	-0.963092000
6	6.358566000	-0.269533000	0.825046000
6	8.105728000	1.477618000	1.316621000
6	7.804695000	0.162404000	0.549630000
6	6.273753000	3.954633000	-1.045927000
6	4.671501000	3.231258000	0.742306000
6	4.539142000	2.214503000	-1.547258000
6	4.830827000	3.505670000	-0.763136000
1	9.536866000	1.094002000	-2.320339000
1	10.732569000	2.533558000	-0.672615000
1	9.763779000	2.837057000	1.604739000
1	10.214593000	-1.117538000	-1.386207000
1	11.436633000	0.106401000	-1.034278000
1	8.677078000	-1.139590000	2.044007000
1	8.583986000	-1.854690000	0.433719000

1	10.442351000	0.632023000	2.553520000
1	11.571343000	1.141243000	1.296016000
1	10.945843000	-1.262128000	1.000651000
1	8.932272000	4.232356000	-0.356321000
1	8.839179000	3.517250000	-1.966625000
1	7.091234000	1.744768000	-2.464852000
1	7.317842000	3.485530000	1.455063000
1	5.540997000	1.936328000	2.248854000
1	4.345297000	0.496772000	0.601130000
1	5.314090000	0.193272000	-1.676224000
1	7.760025000	-0.455201000	-1.526548000
1	6.145595000	-1.202027000	0.284836000
1	6.238686000	-0.486920000	1.895139000
1	7.986635000	1.285561000	2.393367000
1	6.493873000	4.885021000	-0.505204000
1	6.400783000	4.169921000	-2.115492000
1	4.863269000	4.147868000	1.314721000
1	3.641231000	2.923929000	0.962793000
1	4.635516000	2.398307000	-2.625005000
1	3.506518000	1.889088000	-1.367501000
1	4.132018000	4.292459000	-1.072136000
6	-5.651545000	-2.129945000	-1.173101000
6	-5.373613000	-0.824097000	-0.396324000
6	-5.519342000	-1.114391000	1.113762000
6	-4.671500000	-3.231258000	-0.742306000
6	-6.273753000	-3.954633000	1.045927000
6	-4.539142000	-2.214503000	1.547258000
6	-4.830827000	-3.505670000	0.763136000
6	-6.358566000	0.269534000	-0.825046000
6	-8.105731000	-1.477617000	-1.316621000
6	-7.804692000	-0.162405000	-0.549630000
6	-7.973942000	-0.465237000	0.963092000
6	-9.426319000	-0.900384000	1.244586000
6	-9.704251000	-2.206234000	0.467810000
6	-9.558522000	-1.915939000	-1.042277000
6	-7.103922000	-2.565093000	-0.891607000
6	-8.719298000	-3.299863000	0.896531000
6	-6.972133000	-1.552713000	1.388106000
6	-7.273172000	-2.867925000	0.621115000
6	-8.804111000	0.924303000	-0.974442000
6	-10.406363000	0.200927000	0.813791000
6	-10.538722000	-0.815827000	-1.475773000
6	-10.247037000	0.475340000	-0.691650000
1	-5.540997000	-1.936328000	-2.248854000
1	-4.345297000	-0.496772000	-0.601130000
1	-5.314090000	-0.193272000	1.676224000
1	-4.863269000	-4.147868000	-1.314721000
1	-3.641230000	-2.923929000	-0.962793000
1	-6.400783000	-4.169921000	2.115492000
1	-6.493873000	-4.885021000	0.505204000

1	-4.635515000	-2.398307000	2.625005000
1	-3.506517000	-1.889088000	1.367501000
1	-4.132018000	-4.292459000	1.072136000
1	-6.145595000	1.202027000	-0.284836000
1	-6.238686000	0.486920000	-1.895139000
1	-7.986630000	-1.285562000	-2.393367000
1	-7.760022000	0.455200000	1.526548000
1	-9.536867000	-1.094002000	2.320339000
1	-10.732567000	-2.533558000	0.672615000
1	-9.763775000	-2.837058000	-1.604739000
1	-7.317842000	-3.485530000	-1.455063000
1	-8.932269000	-4.232357000	0.356321000
1	-8.839179000	-3.517250000	1.966625000
1	-7.091234000	-1.744768000	2.464852000
1	-8.583991000	1.854691000	-0.433719000
1	-8.677081000	1.139591000	-2.044006000
1	-10.214595000	1.117538000	1.386207000
1	-11.436634000	-0.106401000	1.034278000
1	-10.442348000	-0.632023000	-2.553520000
1	-11.571347000	-1.141242000	-1.296016000
1	-10.945846000	1.262129000	-1.000651000
6	4.147428000	-4.563973000	-1.429278000
6	4.425360000	-3.258125000	-0.652501000
6	4.279631000	-3.548418000	0.857586000
6	5.127473000	-5.665285000	-0.998483000
6	3.525221000	-6.388661000	0.789751000
6	5.259832000	-4.648531000	1.291082000
6	4.968147000	-5.939697000	0.506959000
6	3.440407000	-2.164494000	-1.081223000
6	1.693243000	-3.911645000	-1.572798000
6	1.994282000	-2.596432000	-0.805807000
6	1.825032000	-2.899265000	0.706916000
6	0.372655000	-3.334412000	0.988409000
6	0.094722000	-4.640261000	0.211633000
6	0.240452000	-4.349967000	-1.298454000
6	2.695051000	-4.999120000	-1.147784000
6	1.079676000	-5.733891000	0.640355000
6	2.826840000	-3.986740000	1.131929000
6	2.525801000	-5.301952000	0.364939000
6	0.994862000	-1.509724000	-1.230619000
6	-0.607390000	-2.233101000	0.557615000
6	-0.739749000	-3.249854000	-1.731950000
6	-0.448064000	-1.958687000	-0.947827000
1	4.257976000	-4.370355000	-2.505031000
1	5.453676000	-2.930799000	-0.857307000
1	4.484884000	-2.627299000	1.420047000
1	4.935705000	-6.581896000	-1.570898000
1	6.157742000	-5.357956000	-1.218969000
1	3.398190000	-6.603949000	1.859315000
1	3.305100000	-7.319048000	0.249028000

1	5.163458000	-4.832335000	2.368828000
1	6.292452000	-4.323115000	1.111324000
1	5.666953000	-6.726486000	0.815960000
1	3.653379000	-1.232001000	-0.541013000
1	3.560288000	-1.947107000	-2.151316000
1	1.812344000	-3.719590000	-2.649544000
1	2.038952000	-1.978827000	1.270371000
1	0.262107000	-3.528029000	2.064163000
1	-0.933593000	-4.967586000	0.416438000
1	0.035199000	-5.271085000	-1.860916000
1	2.481131000	-5.919558000	-1.711239000
1	0.866704000	-6.666384000	0.100144000
1	0.959795000	-5.951277000	1.710448000
1	2.707739000	-4.178795000	2.208675000
1	1.214983000	-0.579337000	-0.689896000
1	1.121893000	-1.294436000	-2.300183000
1	-0.415622000	-1.316489000	1.130030000
1	-1.637660000	-2.540429000	0.778101000
1	-0.643375000	-3.066050000	-2.809697000
1	-1.772373000	-3.575269000	-1.552193000
1	-1.146872000	-1.171899000	-1.256828000

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**Type B (+5°) on Au(111)**

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6	9.438932000	0.711618000	1.517093000
6	9.090597000	-0.590899000	0.763449000
6	9.316887000	-0.356248000	-0.746386000
6	10.896871000	1.114261000	1.250162000
6	10.159872000	2.459764000	-0.733451000
6	10.774683000	0.045133000	-1.015991000
6	11.102793000	1.342735000	-0.257299000
6	7.632817000	-0.984565000	1.027774000
6	7.012385000	1.442009000	1.299009000
6	6.677327000	0.120060000	0.558152000
6	6.890723000	0.377481000	-0.957394000
6	5.932441000	1.487737000	-1.433859000
6	6.280776000	2.790254000	-0.680214000
6	6.054486000	2.555604000	0.829620000
6	8.480650000	1.821875000	1.040628000
6	7.738556000	3.183920000	-0.944540000
6	8.358988000	0.757346000	-1.215775000
6	8.694046000	2.079296000	-0.474918000
6	5.211500000	-0.260408000	0.816685000
6	4.474502000	1.085094000	-1.166928000
6	4.596690000	2.154222000	1.099225000
6	4.268580000	0.856621000	0.340533000
1	9.290298000	0.552181000	2.593866000
1	9.758296000	-1.393044000	1.105884000
1	9.080827000	-1.280662000	-1.291076000
1	11.140626000	2.028398000	1.806531000
1	11.574638000	0.329051000	1.608766000

1	10.305167000	2.646602000	-1.806034000
1	10.391104000	3.398537000	-0.212212000
1	10.930374000	0.188715000	-2.092910000
1	11.450277000	-0.759096000	-0.697699000
1	12.143388000	1.631015000	-0.449411000
1	7.394397000	-1.921382000	0.505990000
1	7.480335000	-1.169439000	2.099828000
1	6.871640000	1.279508000	2.378006000
1	6.662445000	-0.550923000	-1.501825000
1	6.081075000	1.647174000	-2.510632000
1	5.613077000	3.592399000	-1.022650000
1	6.290546000	3.480017000	1.374311000
1	8.708928000	2.750278000	1.585060000
1	7.976976000	4.120737000	-0.422756000
1	7.891038000	3.368794000	-2.016594000
1	8.499732000	0.919847000	-2.294771000
1	4.980269000	-1.199182000	0.295447000
1	5.066206000	-0.447247000	1.889268000
1	4.230747000	0.170957000	-1.723297000
1	3.796735000	1.870304000	-1.525532000
1	4.440999000	2.010640000	2.176145000
1	3.921096000	2.958451000	0.780933000
1	3.227985000	0.568340000	0.532646000
6	-0.251332000	3.558782000	1.566683000
6	-0.599666000	2.256265000	0.813038000
6	-0.373376000	2.490915000	-0.696796000
6	1.206607000	3.961425000	1.299752000
6	0.469609000	5.306927000	-0.683861000
6	1.084419000	2.892296000	-0.966401000
6	1.412530000	4.189898000	-0.207709000
6	-2.057446000	1.862599000	1.077364000
6	-2.677876000	4.289171000	1.348599000
6	-3.012939000	2.967224000	0.607742000
6	-2.799538000	3.224643000	-0.907804000
6	-3.757824000	4.334901000	-1.384269000
6	-3.409486000	5.637417000	-0.630625000
6	-3.635781000	5.402768000	0.879210000
6	-1.209613000	4.669038000	1.090218000
6	-1.951711000	6.031084000	-0.894950000
6	-1.331275000	3.604510000	-1.166185000
6	-0.996217000	4.926459000	-0.425328000
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6	-5.215763000	3.932258000	-1.117338000
6	-5.093575000	5.001386000	1.148815000
6	-5.421682000	3.703783000	0.390123000
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1	-0.609437000	1.566501000	-1.241487000
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1	1.884375000	3.176214000	1.658356000

1	0.614903000	5.493765000	-1.756444000
1	0.700841000	6.245701000	-0.162623000
1	1.240110000	3.035878000	-2.043321000
1	1.760014000	2.088067000	-0.648109000
1	2.453125000	4.478179000	-0.399822000
1	-2.295867000	0.925781000	0.555580000
1	-2.209929000	1.677725000	2.149418000
1	-2.818626000	4.126672000	2.427595000
1	-3.027816000	2.296239000	-1.452236000
1	-3.609186000	4.494337000	-2.461042000
1	-4.077182000	6.439561000	-0.973060000
1	-3.399720000	6.327181000	1.423900000
1	-0.981335000	5.597441000	1.634649000
1	-1.713291000	6.967901000	-0.373166000
1	-1.799224000	6.215957000	-1.967005000
1	-1.190531000	3.767010000	-2.245182000
1	-4.709996000	1.647982000	0.345036000
1	-4.624056000	2.399916000	1.938858000
1	-5.459516000	3.018120000	-1.673708000
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1	-5.249259000	4.857802000	2.225734000
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6	3.757821000	-4.334899000	1.384270000
6	3.409487000	-5.637417000	0.630625000
6	3.635778000	-5.402767000	-0.879210000
6	5.215761000	-3.932257000	1.117338000
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6	5.093573000	-5.001385000	-1.148815000
6	5.421683000	-3.703783000	-0.390123000
6	1.951707000	-6.031084000	0.894950000
6	1.331275000	-3.604510000	1.166185000
6	0.996216000	-4.926458000	0.425328000
6	1.209613000	-4.669037000	-1.090218000
6	0.251332000	-3.558782000	-1.566683000
6	0.599666000	-2.256264000	-0.813038000
6	0.373375000	-2.490915000	0.696796000
6	2.799540000	-3.224644000	0.907804000
6	2.057446000	-1.862598000	-1.077364000
6	2.677878000	-4.289172000	-1.348599000
6	3.012936000	-2.967223000	-0.607742000
6	-0.469609000	-5.306926000	0.683861000
6	-1.206607000	-3.961425000	-1.299752000
6	-1.084419000	-2.892296000	0.966401000
6	-1.412530000	-4.189898000	0.207709000
1	3.609187000	-4.494337000	2.461042000
1	4.077185000	-6.439563000	0.973060000
1	3.399716000	-6.327180000	-1.423900000
1	5.459516000	-3.018120000	1.673708000
1	5.893529000	-4.717467000	1.475942000

1	4.624057000	-2.399916000	-1.938858000
1	4.709993000	-1.647981000	-0.345036000
1	5.249263000	-4.857803000	-2.225734000
1	5.769167000	-5.805614000	-0.830523000
1	6.462278000	-3.415503000	-0.582235000
1	1.713287000	-6.967900000	0.373166000
1	1.799225000	-6.215958000	1.967005000
1	1.190531000	-3.767010000	2.245182000
1	0.981335000	-5.597442000	-1.634649000
1	0.399966000	-3.399344000	-2.643455000
1	-0.068032000	-1.454119000	-1.155474000
1	0.609436000	-1.566502000	1.241487000
1	3.027818000	-2.296240000	1.452236000
1	2.295866000	-0.925782000	-0.555580000
1	2.209928000	-1.677724000	-2.149418000
1	2.818623000	-4.126671000	-2.427595000
1	-0.700841000	-6.245700000	0.162623000
1	-0.614903000	-5.493766000	1.756444000
1	-1.450363000	-4.875561000	-1.856121000
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1	-1.760014000	-2.088067000	0.648109000
1	-2.453126000	-4.478178000	0.399822000
6	-5.932443000	-1.487736000	1.433859000
6	-6.280781000	-2.790253000	0.680214000
6	-6.054486000	-2.555603000	-0.829620000
6	-4.474504000	-1.085093000	1.166928000
6	-5.211499000	0.260407000	-0.816685000
6	-4.596692000	-2.154222000	-1.099225000
6	-4.268576000	-0.856621000	-0.340533000
6	-7.738556000	-3.183920000	0.944540000
6	-8.358989000	-0.757346000	1.215775000
6	-8.694043000	-2.079296000	0.474918000
6	-8.480651000	-1.821874000	-1.040628000
6	-9.438928000	-0.711620000	-1.517093000
6	-9.090600000	0.590900000	-0.763448000
6	-9.316884000	0.356247000	0.746386000
6	-6.890720000	-0.377482000	0.957394000
6	-7.632815000	0.984565000	-1.027774000
6	-7.012382000	-1.442010000	-1.299009000
6	-6.677328000	-0.120060000	-0.558152000
6	-10.159872000	-2.459763000	0.733451000
6	-10.896867000	-1.114263000	-1.250162000
6	-10.774679000	-0.045134000	1.015991000
6	-11.102795000	-1.342735000	0.257299000
1	-6.081071000	-1.647175000	2.510632000
1	-5.613075000	-3.592400000	1.022650000
1	-6.290547000	-3.480016000	-1.374311000
1	-4.230751000	-0.170956000	1.723297000
1	-3.796736000	-1.870303000	1.525532000

1	-5.066211000	0.447249000	-1.889268000
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1	-4.440998000	-2.010640000	-2.176145000
1	-3.921097000	-2.958451000	-0.780933000
1	-3.227985000	-0.568340000	-0.532646000
1	-7.976976000	-4.120737000	0.422756000
1	-7.891043000	-3.368793000	2.016594000
1	-8.499730000	-0.919848000	2.294771000
1	-8.708929000	-2.750278000	-1.585060000
1	-9.290300000	-0.552181000	-2.593866000
1	-9.758296000	1.393044000	-1.105884000
1	-9.080824000	1.280660000	1.291076000
1	-6.662441000	0.550923000	1.501825000
1	-7.394395000	1.921381000	-0.505990000
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1	-6.871641000	-1.279508000	-2.378006000
1	-10.391100000	-3.398538000	0.212212000
1	-10.305170000	-2.646602000	1.806034000
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1	-11.574635000	-0.329053000	-1.608766000
1	-10.930373000	-0.188716000	2.092910000
1	-11.450279000	0.759096000	0.697699000
1	-12.143392000	-1.631014000	0.449411000

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#### Type B (-5°) on Au(111)

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6	5.639785000	-1.580094000	-1.017157000
6	6.077761000	-2.858454000	-0.268933000
6	6.082143000	-2.559361000	1.246453000
6	4.243744000	-1.137428000	-0.554476000
6	5.287009000	0.270555000	1.239248000
6	4.686624000	-2.117852000	1.711807000
6	4.267823000	-0.845016000	0.955807000
6	7.474162000	-3.292045000	-0.729396000
6	8.081958000	-0.891372000	-1.192124000
6	8.504625000	-2.189383000	-0.453745000
6	8.522933000	-1.867578000	1.064408000
6	9.557255000	-0.759074000	1.346168000
6	9.119280000	0.519286000	0.597944000
6	9.114898000	0.220193000	-0.917441000
6	6.674107000	-0.471590000	-0.735397000
6	7.722879000	0.952877000	1.058408000
6	7.115082000	-1.447796000	1.521135000
6	6.692416000	-0.149785000	0.782756000
6	9.910032000	-2.609723000	-0.910237000
6	10.953297000	-1.201740000	0.883488000
6	10.510417000	-0.221316000	-1.382796000
6	10.929217000	-1.494152000	-0.626796000
1	5.624166000	-1.785237000	-2.096335000
1	5.355115000	-3.659766000	-0.474370000
1	6.383410000	-3.466011000	1.788831000

1	3.932982000	-0.241351000	-1.106820000
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1	4.695061000	-1.928397000	2.792846000
1	3.959736000	-2.920123000	1.531484000
1	3.271656000	-0.528107000	1.287579000
1	7.774174000	-4.212046000	-0.209474000
1	7.462686000	-3.522491000	-1.803404000
1	8.058163000	-1.099504000	-2.272201000
1	8.816409000	-2.778066000	1.607854000
1	9.572874000	-0.553931000	2.425347000
1	9.841925000	1.320598000	0.803381000
1	8.813630000	1.126844000	-1.459820000
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1	7.422866000	1.872878000	0.538486000
1	7.734354000	1.183323000	2.132415000
1	7.138877000	-1.239664000	2.601213000
1	10.202828000	-3.531554000	-0.389705000
1	9.891343000	-2.842006000	-1.983618000
1	11.264058000	-2.097817000	1.435831000
1	11.688063000	-0.416909000	1.104126000
1	10.501980000	-0.410771000	-2.463835000
1	11.237304000	0.580955000	-1.202473000
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6	-4.391830000	-2.612496000	1.104929000
6	-4.992218000	-5.000904000	1.577488000
6	-5.411019000	-3.728068000	0.821488000
6	-2.204681000	-6.175097000	-0.863716000
6	-1.596883000	-3.774424000	-1.326443000
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6	0.231191000	-5.492774000	-1.044556000
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1	-1.620679000	-3.982555000	-2.406521000
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1	0.163084000	-1.562453000	0.669062000
1	-0.865211000	-1.756208000	-1.594139000
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1	0.212502000	-5.725057000	-2.117938000
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6	0.563944000	2.662858000	1.051760000
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6	2.986426000	3.032836000	-0.648437000
6	3.004734000	3.354641000	0.869716000
6	4.039056000	4.463145000	1.151476000
6	3.601080000	5.741507000	0.403252000
6	3.596698000	5.442412000	-1.112133000
6	1.155908000	4.750629000	-0.930089000
6	2.204680000	6.175097000	0.863716000
6	1.596883000	3.774423000	1.326443000
6	1.174216000	5.072434000	0.588064000
6	4.391833000	2.612497000	-1.104929000
6	5.435098000	4.020480000	0.688795000
6	4.992218000	5.000903000	-1.577488000
6	5.411018000	3.728067000	-0.821488000
1	0.105967000	3.436981000	-2.291027000
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1	0.865211000	1.756208000	1.594139000

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1	-0.212502000	5.725057000	2.117938000
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1	-2.246543000	4.694112000	1.092887000
1	2.255975000	1.010173000	-0.404166000
1	1.944487000	1.699728000	-1.998096000
1	2.539964000	4.122715000	-2.466894000
1	3.298210000	2.444154000	1.413162000
1	4.054675000	4.668289000	2.230654000
1	4.323726000	6.542817000	0.608689000
1	3.295431000	6.349063000	-1.654512000
1	0.862433000	5.661117000	-1.473535000
1	1.904667000	7.095097000	0.343793000
1	2.216155000	6.405542000	1.937723000
1	1.620678000	3.982555000	2.406521000
1	4.684629000	1.690665000	-0.584397000
1	4.373144000	2.380213000	-2.178311000
1	5.745859000	3.124402000	1.241139000
1	6.169864000	4.805310000	0.909434000
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1	6.407185000	3.411159000	-1.153259000
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6	-10.953298000	1.201740000	-0.883488000
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6	-10.929218000	1.494152000	0.626796000
6	-7.722880000	-0.952878000	-1.058408000
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6	-6.692413000	0.149786000	-0.782756000
6	-6.674108000	0.471590000	0.735397000
6	-5.639788000	1.580093000	1.017157000
6	-6.077760000	2.858456000	0.268933000
6	-6.082143000	2.559361000	-1.246453000
6	-8.522932000	1.867578000	-1.064408000
6	-7.474161000	3.292046000	0.729396000
6	-8.081955000	0.891373000	1.192124000
6	-8.504628000	2.189382000	0.453745000
6	-5.287011000	-0.270556000	-1.239248000
6	-4.243743000	1.137429000	0.554476000
6	-4.686624000	2.117852000	-1.711807000
6	-4.267823000	0.845016000	-0.955807000
1	-9.572873000	0.553930000	-2.425347000
1	-9.841927000	-1.320599000	-0.803382000
1	-8.813634000	-1.126845000	1.459820000

1	-11.264057000	2.097817000	-1.435831000
1	-11.688062000	0.416909000	-1.104126000
1	-9.891340000	2.842007000	1.983618000
1	-10.202823000	3.531555000	0.389705000
1	-10.501982000	0.410770000	2.463835000
1	-11.237301000	-0.580954000	1.202473000
1	-11.925381000	1.811061000	0.958567000
1	-7.422869000	-1.872879000	-0.538486000
1	-7.734355000	-1.183323000	-2.132415000
1	-7.138873000	1.239666000	-2.601213000
1	-6.380629000	-0.438897000	1.278843000
1	-5.624168000	1.785237000	2.096335000
1	-5.355113000	3.659767000	0.474370000
1	-6.383407000	3.466013000	-1.788831000
1	-8.816412000	2.778065000	-1.607854000
1	-7.774171000	4.212047000	0.209474000
1	-7.462686000	3.522491000	1.803404000
1	-8.058168000	1.099502000	2.272201000
1	-4.994217000	-1.192387000	-0.718716000
1	-5.305700000	-0.502839000	-2.312630000
1	-3.932984000	0.241351000	1.106820000
1	-3.508978000	1.922259000	0.775114000
1	-4.695059000	1.928398000	-2.792846000
1	-3.959736000	2.920123000	-1.531484000
1	-3.271657000	0.528107000	-1.287579000

#### Type A (+5°) on Cu(111)

6	4.000372000	-4.538879000	-1.573725000
6	4.362942000	-3.238169000	-0.823683000
6	4.453841000	-3.554507000	0.685468000
6	5.058959000	-5.621471000	-1.316142000
6	3.762321000	-6.411513000	0.679560000
6	5.512964000	-4.635936000	0.945719000
6	5.135358000	-5.922209000	0.190763000
6	3.299992000	-2.163410000	-1.078618000
6	1.538577000	-3.946464000	-1.333371000
6	1.922292000	-2.635666000	-0.596313000
6	1.990629000	-2.965169000	0.918758000
6	0.607742000	-3.440881000	1.407955000
6	0.245171000	-4.741591000	0.657913000
6	0.154273000	-4.425253000	-0.851238000
6	2.617485000	-5.014591000	-1.084528000
6	1.308121000	-5.816351000	0.912848000
6	3.069536000	-4.033297000	1.167601000
6	2.685822000	-5.344094000	0.430543000
6	0.845793000	-1.568247000	-0.845330000
6	-0.450845000	-2.358289000	1.150372000
6	-0.904850000	-3.343824000	-1.111488000
6	-0.527245000	-2.057552000	-0.356532000
1	3.942571000	-4.326534000	-2.650070000

1	5.340791000	-2.882049000	-1.175127000
1	4.720887000	-2.636997000	1.227514000
1	4.803631000	-6.533988000	-1.869976000
1	6.036819000	-5.285057000	-1.683750000
1	3.803388000	-6.645842000	1.751874000
1	3.484079000	-7.338985000	0.161071000
1	5.584853000	-4.838147000	2.022080000
1	6.498901000	-4.281991000	0.618347000
1	5.890481000	-6.695676000	0.376207000
1	3.571044000	-1.234004000	-0.559519000
1	3.251732000	-1.927153000	-2.150338000
1	1.489113000	-3.735449000	-2.412016000
1	2.266405000	-2.048136000	1.460466000
1	0.665543000	-3.653227000	2.484300000
1	-0.732677000	-5.097711000	1.009357000
1	-0.112773000	-5.342763000	-1.393284000
1	2.341708000	-5.931624000	-1.626236000
1	1.037070000	-6.745757000	0.393749000
1	1.356382000	-6.052607000	1.984568000
1	3.119000000	-4.244311000	2.246246000
1	1.124034000	-0.640775000	-0.326841000
1	0.804726000	-1.333918000	-1.917644000
1	-0.195518000	-1.445772000	1.704206000
1	-1.428706000	-2.694703000	1.517980000
1	-0.976739000	-3.141614000	-2.187850000
1	-1.890787000	-3.697769000	-0.784117000
1	-1.282367000	-1.284084000	-0.541977000
6	-5.924784000	-2.083328000	-1.534199000
6	-5.562213000	-0.782618000	-0.784157000
6	-5.471315000	-1.098956000	0.724994000
6	-4.866197000	-3.165920000	-1.276616000
6	-6.162836000	-3.955961000	0.719086000
6	-4.412192000	-2.180385000	0.985245000
6	-4.789797000	-3.466657000	0.230289000
6	-6.625164000	0.292142000	-1.039092000
6	-8.386575000	-1.490913000	-1.293845000
6	-8.002866000	-0.180114000	-0.556787000
6	-7.934523000	-0.509619000	0.958284000
6	-9.317415000	-0.985329000	1.447481000
6	-9.679983000	-2.286040000	0.697439000
6	-9.770885000	-1.969701000	-0.811712000
6	-7.307671000	-2.559040000	-1.045002000
6	-8.617037000	-3.360798000	0.952374000
6	-6.855619000	-1.577745000	1.207127000
6	-7.239334000	-2.888543000	0.470069000
6	-9.079358000	0.887303000	-0.805804000
6	-10.376002000	0.097263000	1.189898000
6	-10.830007000	-0.888272000	-1.071962000
6	-10.452398000	0.397999000	-0.317007000
1	-5.982585000	-1.870982000	-2.610544000

1	-4.584365000	-0.426498000	-1.135601000
1	-5.204269000	-0.181446000	1.267040000
1	-5.121525000	-4.078436000	-1.830450000
1	-3.888337000	-2.829506000	-1.644224000
1	-6.121768000	-4.190290000	1.791400000
1	-6.441077000	-4.883433000	0.200597000
1	-4.340304000	-2.382595000	2.061606000
1	-3.426256000	-1.826439000	0.657873000
1	-4.034675000	-4.240125000	0.415733000
1	-6.354112000	1.221548000	-0.519993000
1	-6.673424000	0.528398000	-2.110812000
1	-8.436045000	-1.279897000	-2.372490000
1	-7.658747000	0.407414000	1.499992000
1	-9.259610000	-1.197676000	2.523826000
1	-10.657838000	-2.642158000	1.048883000
1	-10.037931000	-2.887211000	-1.353758000
1	-7.583448000	-3.476072000	-1.586710000
1	-8.888089000	-4.290205000	0.433275000
1	-8.568772000	-3.597056000	2.024094000
1	-6.806155000	-1.788760000	2.285772000
1	-8.801123000	1.814776000	-0.287315000
1	-9.120428000	1.121633000	-1.878118000
1	-10.120673000	1.009779000	1.743732000
1	-11.353862000	-0.239151000	1.557506000
1	-10.901899000	-0.686061000	-2.148324000
1	-11.815940000	-1.242218000	-0.744591000
1	-11.207522000	1.171467000	-0.502451000
6	9.317414000	0.985329000	-1.447481000
6	9.679985000	2.286040000	-0.697439000
6	9.770883000	1.969701000	0.811712000
6	10.376000000	-0.097262000	-1.189898000
6	9.079362000	-0.887304000	0.805804000
6	10.830006000	0.888273000	1.071962000
6	10.452400000	-0.398000000	0.317007000
6	8.617034000	3.360800000	-0.952374000
6	6.855620000	1.577745000	-1.207127000
6	7.239334000	2.888543000	-0.470069000
6	7.307671000	2.559039000	1.045002000
6	5.924784000	2.083327000	1.534199000
6	5.562213000	0.782617000	0.784157000
6	5.471315000	1.098956000	-0.724994000
6	7.934527000	0.509617000	-0.958284000
6	6.625164000	-0.292142000	1.039092000
6	8.386578000	1.490912000	1.293845000
6	8.002864000	0.180114000	0.556787000
6	6.162836000	3.955961000	-0.719086000
6	4.866197000	3.165920000	1.276616000
6	4.412192000	2.180385000	-0.985245000
6	4.789798000	3.466658000	-0.230289000
1	9.259613000	1.197676000	-2.523826000

1	10.657833000	2.642160000	-1.048883000
1	10.037929000	2.887211000	1.353758000
1	10.120674000	-1.009778000	-1.743732000
1	11.353861000	0.239151000	-1.557506000
1	9.120430000	-1.121633000	1.878118000
1	8.801121000	-1.814775000	0.287315000
1	10.901894000	0.686062000	2.148324000
1	11.815943000	1.242218000	0.744591000
1	11.207524000	-1.171467000	0.502451000
1	8.888087000	4.290205000	-0.433275000
1	8.568774000	3.597056000	-2.024094000
1	6.806155000	1.788760000	-2.285772000
1	7.583448000	3.476073000	1.586710000
1	5.982586000	1.870982000	2.610544000
1	4.584366000	0.426497000	1.135601000
1	5.204270000	0.181446000	-1.267040000
1	7.658751000	-0.407416000	-1.499992000
1	6.354112000	-1.221548000	0.519993000
1	6.673424000	-0.528398000	2.110812000
1	8.436042000	1.279898000	2.372490000
1	6.441077000	4.883433000	-0.200597000
1	6.121768000	4.190291000	-1.791400000
1	5.121524000	4.078436000	1.830450000
1	3.888337000	2.829506000	1.644224000
1	4.340304000	2.382595000	-2.061606000
1	3.426256000	1.826440000	-0.657873000
1	4.034675000	4.240124000	-0.415733000
6	-0.607742000	3.440881000	-1.407955000
6	-0.245171000	4.741592000	-0.657913000
6	-0.154272000	4.425253000	0.851238000
6	0.450845000	2.358289000	-1.150372000
6	-0.845793000	1.568247000	0.845330000
6	0.904850000	3.343824000	1.111488000
6	0.527244000	2.057551000	0.356532000
6	-1.308122000	5.816351000	-0.912848000
6	-3.069537000	4.033297000	-1.167601000
6	-2.685822000	5.344094000	-0.430543000
6	-2.617485000	5.014591000	1.084528000
6	-4.000372000	4.538879000	1.573725000
6	-4.362943000	3.238169000	0.823683000
6	-4.453841000	3.554508000	-0.685468000
6	-1.990629000	2.965169000	-0.918758000
6	-3.299993000	2.163409000	1.078618000
6	-1.538577000	3.946464000	1.333371000
6	-1.922292000	2.635666000	0.596313000
6	-3.762320000	6.411512000	-0.679560000
6	-5.058959000	5.621472000	1.316142000
6	-5.512964000	4.635937000	-0.945719000
6	-5.135359000	5.922209000	-0.190763000
1	-0.665543000	3.653227000	-2.484300000

1	0.732677000	5.097712000	-1.009357000
1	0.112773000	5.342763000	1.393284000
1	0.195519000	1.445773000	-1.704206000
1	1.428705000	2.694703000	-1.517980000
1	-0.804726000	1.333918000	1.917644000
1	-1.124034000	0.640776000	0.326841000
1	0.976739000	3.141614000	2.187850000
1	1.890787000	3.697769000	0.784117000
1	1.282367000	1.284085000	0.541977000
1	-1.037070000	6.745756000	-0.393749000
1	-1.356382000	6.052607000	-1.984568000
1	-3.119001000	4.244311000	-2.246246000
1	-2.341708000	5.931625000	1.626236000
1	-3.942571000	4.326534000	2.650070000
1	-5.340791000	2.882049000	1.175127000
1	-4.720887000	2.636998000	-1.227514000
1	-2.266405000	2.048136000	-1.460466000
1	-3.571044000	1.234003000	0.559519000
1	-3.251732000	1.927153000	2.150338000
1	-1.489113000	3.735449000	2.412016000
1	-3.484079000	7.338984000	-0.161071000
1	-3.803388000	6.645842000	-1.751874000
1	-4.803632000	6.533987000	1.869976000
1	-6.036821000	5.285057000	1.683750000
1	-5.584852000	4.838147000	-2.022080000
1	-6.498898000	4.281990000	-0.618347000
1	-5.890480000	6.695676000	-0.376207000

#### Type A (-5°) on Cu(111)

6	0.411404000	-3.372862000	-0.988969000
6	0.134663000	-4.679562000	-0.213201000
6	0.280673000	-4.390433000	1.297083000
6	-0.569292000	-2.272617000	-0.556931000
6	1.033019000	-1.549593000	1.231392000
6	-0.700178000	-3.291391000	1.731820000
6	-0.409675000	-1.999356000	0.948689000
6	1.120263000	-5.772124000	-0.643160000
6	2.866012000	-4.023304000	-1.133831000
6	2.566167000	-5.339377000	-0.367849000
6	2.735689000	-5.037694000	1.145073000
6	4.187844000	-4.601740000	1.426463000
6	4.464586000	-3.295040000	0.650695000
6	4.318576000	-3.584168000	-0.859589000
6	1.863559000	-2.936907000	-0.707579000
6	3.478985000	-2.202478000	1.080654000
6	1.733237000	-3.951297000	1.571325000
6	2.033082000	-2.635225000	0.805343000
6	3.566229000	-6.425008000	-0.793898000
6	5.168540000	-5.701984000	0.994425000
6	5.299427000	-4.683211000	-1.294326000

6	5.008924000	-5.975246000	-0.511195000
1	0.300647000	-3.565654000	-2.064849000
1	-0.893484000	-5.007455000	-0.417949000
1	0.076264000	-5.312172000	1.858836000
1	-0.378368000	-1.355388000	-1.128638000
1	-1.599412000	-2.580501000	-0.777343000
1	1.160241000	-1.335113000	2.301095000
1	1.252295000	-0.618593000	0.691380000
1	-0.603587000	-3.108424000	2.809690000
1	-1.732626000	-3.617397000	1.552123000
1	-1.108949000	-1.213330000	1.258577000
1	0.908137000	-6.705223000	-0.103665000
1	1.000192000	-5.988697000	-1.713397000
1	2.746700000	-4.214540000	-2.210699000
1	2.522614000	-5.958759000	1.707824000
1	4.298601000	-4.408947000	2.502343000
1	5.492732000	-2.967147000	0.855443000
1	4.522984000	-2.662430000	-1.421342000
1	2.076635000	-2.015843000	-1.270330000
1	3.691112000	-1.269378000	0.541159000
1	3.599057000	-1.985905000	2.150891000
1	1.852548000	-3.760062000	2.648193000
1	3.346953000	-7.356008000	-0.253886000
1	3.439007000	-6.639489000	-1.863601000
1	4.977617000	-6.619213000	1.566132000
1	6.198661000	-5.394100000	1.214837000
1	5.202836000	-4.866178000	-2.372196000
1	6.331875000	-4.357204000	-1.114629000
1	5.708198000	-6.761272000	-0.821083000
6	-9.510189000	-0.915754000	-1.243023000
6	-9.786934000	-2.222453000	-0.467255000
6	-9.640923000	-1.933324000	1.043028000
6	-10.490888000	0.184492000	-0.810985000
6	-8.888574000	0.907515000	0.977337000
6	-10.621774000	-0.834282000	1.477766000
6	-10.331272000	0.457753000	0.694635000
6	-8.801334000	-3.315014000	-0.897214000
6	-7.055585000	-1.566195000	-1.387885000
6	-7.355430000	-2.882267000	-0.621903000
6	-7.185907000	-2.580585000	0.891019000
6	-5.733752000	-2.144630000	1.172409000
6	-5.457011000	-0.837930000	0.396640000
6	-5.603021000	-1.127059000	-1.113643000
6	-8.058036000	-0.479798000	-0.961633000
6	-6.442611000	0.254631000	0.826600000
6	-8.188356000	-1.494189000	1.317271000
6	-7.888517000	-0.178115000	0.551289000
6	-6.355367000	-3.967899000	-1.047952000
6	-4.753056000	-3.244875000	0.740371000
6	-4.622170000	-2.226101000	-1.548380000

6	-4.912673000	-3.518136000	-0.765249000
1	-9.620948000	-1.108545000	-2.318903000
1	-10.815081000	-2.550345000	-0.672003000
1	-9.845335000	-2.855062000	1.604782000
1	-10.299962000	1.101720000	-1.382692000
1	-11.521007000	-0.123392000	-1.031397000
1	-8.761351000	1.121996000	2.047041000
1	-8.669305000	1.838517000	0.437325000
1	-10.525185000	-0.651314000	2.555636000
1	-11.654228000	-1.160287000	1.298069000
1	-11.030542000	1.243779000	1.004523000
1	-9.013462000	-4.248114000	-0.357719000
1	-8.921404000	-3.531588000	-1.967451000
1	-7.174897000	-1.757430000	-2.464754000
1	-7.398983000	-3.501650000	1.453770000
1	-5.622995000	-1.951838000	2.248288000
1	-4.428864000	-0.510037000	0.601388000
1	-5.398613000	-0.205320000	-1.675396000
1	-7.844964000	0.441267000	-1.524384000
1	-6.230485000	1.187731000	0.287105000
1	-6.322540000	0.471204000	1.896837000
1	-8.069052000	-1.302952000	2.394139000
1	-6.574643000	-4.898899000	-0.507940000
1	-6.482590000	-4.182379000	-2.117656000
1	-4.943980000	-4.162104000	1.312077000
1	-3.722936000	-2.936991000	0.960783000
1	-4.718761000	-2.409069000	-2.626250000
1	-3.589722000	-1.900095000	-1.368684000
1	-4.213399000	-4.304162000	-1.075137000
6	5.733753000	2.144630000	-1.172409000
6	5.457010000	0.837930000	-0.396640000
6	5.603021000	1.127060000	1.113643000
6	4.753056000	3.244875000	-0.740371000
6	6.355367000	3.967900000	1.047952000
6	4.622170000	2.226101000	1.548380000
6	4.912673000	3.518136000	0.765249000
6	6.442612000	-0.254631000	-0.826600000
6	8.188360000	1.494188000	-1.317271000
6	7.888514000	0.178115000	-0.551289000
6	8.058037000	0.479798000	0.961633000
6	9.510192000	0.915752000	1.243023000
6	9.786934000	2.222453000	0.467255000
6	9.640923000	1.933324000	-1.043028000
6	7.185908000	2.580585000	-0.891019000
6	8.801333000	3.315014000	0.897214000
6	7.055585000	1.566196000	1.387885000
6	7.355430000	2.882267000	0.621903000
6	8.888578000	-0.907517000	-0.977337000
6	10.490889000	-0.184492000	0.810985000
6	10.621775000	0.834282000	-1.477766000

6	10.331272000	-0.457754000	-0.694635000
1	5.622995000	1.951838000	-2.248288000
1	4.428864000	0.510038000	-0.601389000
1	5.398613000	0.205321000	1.675396000
1	4.943980000	4.162104000	-1.312077000
1	3.722936000	2.936991000	-0.960783000
1	6.482589000	4.182379000	2.117656000
1	6.574644000	4.898899000	0.507940000
1	4.718760000	2.409069000	2.626250000
1	3.589721000	1.900095000	1.368684000
1	4.213399000	4.304162000	1.075137000
1	6.230484000	-1.187731000	-0.287105000
1	6.322539000	-0.471205000	-1.896837000
1	8.069048000	1.302952000	-2.394139000
1	7.844962000	-0.441267000	1.524384000
1	9.620950000	1.108545000	2.318903000
1	10.815081000	2.550345000	0.672003000
1	9.845332000	2.855062000	-1.604782000
1	7.398983000	3.501650000	-1.453770000
1	9.013460000	4.248115000	0.357719000
1	8.921404000	3.531588000	1.967451000
1	7.174896000	1.757430000	2.464754000
1	8.669301000	-1.838515000	-0.437326000
1	8.761356000	-1.121996000	-2.047041000
1	10.299964000	-1.101721000	1.382692000
1	11.521009000	0.123392000	1.031397000
1	10.525184000	0.651314000	-2.555636000
1	11.654223000	1.160287000	-1.298069000
1	11.030546000	-1.243780000	-1.004523000
6	-4.187845000	4.601739000	-1.426463000
6	-4.464586000	3.295039000	-0.650695000
6	-4.318575000	3.584169000	0.859589000
6	-5.168541000	5.701984000	-0.994425000
6	-3.566230000	6.425009000	0.793898000
6	-5.299427000	4.683211000	1.294326000
6	-5.008925000	5.975246000	0.511195000
6	-3.478986000	2.202479000	-1.080654000
6	-1.733237000	3.951297000	-1.571325000
6	-2.033082000	2.635225000	-0.805343000
6	-1.863560000	2.936907000	0.707579000
6	-0.411405000	3.372862000	0.988969000
6	-0.134663000	4.679563000	0.213201000
6	-0.280673000	4.390433000	-1.297083000
6	-2.735690000	5.037694000	-1.145073000
6	-1.120264000	5.772123000	0.643160000
6	-2.866012000	4.023305000	1.133831000
6	-2.566168000	5.339377000	0.367849000
6	-1.033019000	1.549593000	-1.231392000
6	0.569292000	2.272618000	0.556931000
6	0.700177000	3.291391000	-1.731820000

6	0.409675000	1.999356000	-0.948689000
1	-4.298602000	4.408948000	-2.502343000
1	-5.492733000	2.967147000	-0.855443000
1	-4.522984000	2.662430000	1.421342000
1	-4.977618000	6.619213000	-1.566132000
1	-6.198659000	5.394100000	-1.214837000
1	-3.439008000	6.639489000	1.863601000
1	-3.346954000	7.356008000	0.253886000
1	-5.202836000	4.866178000	2.372196000
1	-6.331880000	4.357205000	1.114629000
1	-5.708195000	6.761271000	0.821083000
1	-3.691112000	1.269378000	-0.541159000
1	-3.599057000	1.985905000	-2.150891000
1	-1.852548000	3.760061000	-2.648193000
1	-2.076636000	2.015842000	1.270330000
1	-0.300647000	3.565654000	2.064849000
1	0.893483000	5.007455000	0.417949000
1	-0.076265000	5.312172000	-1.858836000
1	-2.522614000	5.958760000	-1.707824000
1	-0.908137000	6.705224000	0.103665000
1	-1.000192000	5.988697000	1.713397000
1	-2.746701000	4.214540000	2.210699000
1	-1.252296000	0.618594000	-0.691380000
1	-1.160242000	1.335114000	-2.301095000
1	0.378368000	1.355388000	1.128638000
1	1.599412000	2.580501000	0.777343000
1	0.603587000	3.108423000	-2.809690000
1	1.732627000	3.617397000	-1.552123000
1	1.108949000	1.213330000	-1.258577000

#### Type B (+5°) on Cu(111)

6	-9.433618000	0.817496000	-1.518048000
6	-9.085226000	-0.486310000	-0.766662000
6	-9.311505000	-0.254280000	0.743579000
6	-10.891569000	1.219622000	-1.250402000
6	-10.154595000	2.561719000	0.735526000
6	-10.769312000	0.146580000	1.013896000
6	-11.097481000	1.445480000	0.257454000
6	-7.627434000	-0.879464000	-1.031687000
6	-7.007096000	1.547598000	-1.298731000
6	-6.671979000	0.224382000	-0.560166000
6	-6.885365000	0.479173000	0.955825000
6	-5.927119000	1.588639000	1.434198000
6	-6.275512000	2.892445000	0.682812000
6	-6.049232000	2.660415000	-0.827429000
6	-8.475372000	1.926962000	-1.039675000
6	-7.733303000	3.285599000	0.947837000
6	-8.353641000	0.858536000	1.214881000
6	-8.688758000	2.181753000	0.476316000
6	-5.206142000	-0.155584000	-0.819376000

6	-4.469169000	1.186512000	1.166552000
6	-4.591425000	2.259555000	-1.097746000
6	-4.263257000	0.960655000	-0.341304000
1	-9.284992000	0.659927000	-2.595097000
1	-9.752899000	-1.287886000	-1.110476000
1	-9.075404000	-1.179626000	1.286666000
1	-11.135365000	2.134711000	-1.805186000
1	-11.1569312000	0.435008000	-1.610355000
1	-10.299883000	2.746696000	1.808432000
1	-10.385869000	3.501384000	0.215915000
1	-10.924995000	0.288293000	2.091064000
1	-11.444881000	-0.657122000	0.694222000
1	-12.138084000	1.733389000	0.450078000
1	-7.388973000	-1.817173000	-0.511527000
1	-7.474959000	-1.062477000	-2.104061000
1	-6.866359000	1.386970000	-2.378009000
1	-6.657046000	-0.450163000	1.498647000
1	-6.075745000	1.746207000	2.511246000
1	-5.607838000	3.694021000	1.026626000
1	-6.285334000	3.585761000	-1.370517000
1	-8.703691000	2.856297000	-1.582497000
1	-7.971765000	4.223308000	0.427677000
1	-7.885779000	3.468612000	2.020211000
1	-8.494378000	1.019165000	2.294159000
1	-4.974869000	-1.095249000	-0.299765000
1	-5.060855000	-0.340561000	-1.892282000
1	-4.225372000	0.271423000	1.721336000
1	-3.791425000	1.971126000	1.526505000
1	-4.435742000	2.117842000	-2.174915000
1	-3.915857000	3.063257000	-0.778072000
1	-3.222653000	0.672746000	-0.533929000
6	0.375968000	3.700197000	-1.563387000
6	0.724361000	2.396392000	-0.812001000
6	0.498081000	2.628421000	0.698240000
6	-1.081982000	4.102324000	-1.295741000
6	-0.345008000	5.444420000	0.690187000
6	-0.959726000	3.029281000	0.968557000
6	-1.287894000	4.328181000	0.212115000
6	2.182152000	2.003238000	-1.077026000
6	2.802487000	4.430299000	-1.344071000
6	3.137609000	3.107084000	-0.605506000
6	2.924217000	3.361873000	0.910486000
6	3.882468000	4.471341000	1.388859000
6	3.534073000	5.775146000	0.637473000
6	3.760356000	5.543117000	-0.872769000
6	1.334215000	4.809664000	-1.085014000
6	2.076286000	6.168301000	0.902497000
6	1.455945000	3.741238000	1.169542000
6	1.120828000	5.064454000	0.430977000
6	4.603440000	2.727116000	-0.864715000

6	5.340419000	4.069214000	1.121213000
6	5.218162000	5.142257000	-1.143086000
6	5.546327000	3.843356000	-0.386643000
1	0.524594000	3.542629000	-2.640436000
1	0.056687000	1.594815000	-1.155816000
1	0.734183000	1.703076000	1.241327000
1	-1.325779000	5.017413000	-1.850526000
1	-1.759725000	3.317710000	-1.655695000
1	-0.490296000	5.629397000	1.763093000
1	-0.576281000	6.384086000	0.170576000
1	-1.115407000	3.170995000	2.045725000
1	-1.635293000	2.225580000	0.648883000
1	-2.328498000	4.616091000	0.404739000
1	2.420614000	1.065528000	-0.556867000
1	2.334628000	1.820224000	-2.149401000
1	2.943229000	4.269672000	-2.423348000
1	3.152537000	2.432538000	1.453308000
1	3.733838000	4.628908000	2.465907000
1	4.201753000	6.576724000	0.981287000
1	3.524255000	6.468463000	-1.415856000
1	1.105896000	5.738999000	-1.627836000
1	1.837825000	7.106010000	0.382338000
1	1.923806000	6.351313000	1.974872000
1	1.315208000	3.901867000	2.248820000
1	4.834719000	1.787453000	-0.345104000
1	4.748730000	2.542140000	-1.937622000
1	5.584213000	3.154125000	1.675997000
1	6.018162000	4.853828000	1.481166000
1	5.373848000	5.000544000	-2.220254000
1	5.893727000	5.945958000	-0.823412000
1	6.586932000	3.555447000	-0.579268000
6	-3.882467000	-4.471340000	-1.388859000
6	-3.534075000	-5.775147000	-0.637473000
6	-3.760355000	-5.543116000	0.872768000
6	-5.340418000	-4.069214000	-1.121213000
6	-4.603444000	-2.727117000	0.864715000
6	-5.218161000	-5.142257000	1.143086000
6	-5.546329000	-3.843356000	0.386643000
6	-2.076283000	-6.168301000	-0.902497000
6	-1.455945000	-3.741238000	-1.169542000
6	-1.120827000	-5.064454000	-0.430977000
6	-1.334214000	-4.809663000	1.085014000
6	-0.375968000	-3.700197000	1.563387000
6	-0.724360000	-2.396391000	0.812001000
6	-0.498080000	-2.628421000	-0.698240000
6	-2.924221000	-3.361874000	-0.910486000
6	-2.182152000	-2.003237000	1.077026000
6	-2.802490000	-4.430300000	1.344071000
6	-3.137608000	-3.107083000	0.605506000
6	0.345009000	-5.444420000	-0.690187000

6	1.081982000	-4.102324000	1.295741000
6	0.959726000	-3.029281000	-0.968557000
6	1.287894000	-4.328182000	-0.212115000
1	-3.733840000	-4.628909000	-2.465907000
1	-4.201747000	-6.576723000	-0.981287000
1	-3.524252000	-6.468462000	1.415856000
1	-5.584214000	-3.154126000	-1.675997000
1	-6.018161000	-4.853828000	-1.481166000
1	-4.748732000	-2.542140000	1.937622000
1	-4.834717000	-1.787453000	0.345105000
1	-5.373843000	-5.000543000	2.220254000
1	-5.893729000	-5.945959000	0.823412000
1	-6.586933000	-3.555448000	0.579268000
1	-1.837822000	-7.106009000	-0.382338000
1	-1.923808000	-6.351314000	-1.974872000
1	-1.315208000	-3.901867000	-2.248820000
1	-1.105895000	-5.739000000	1.627836000
1	-0.524594000	-3.542629000	2.640436000
1	-0.056688000	-1.594815000	1.155816000
1	-0.734183000	-1.703076000	-1.241327000
1	-3.152540000	-2.432538000	-1.453308000
1	-2.420613000	-1.065528000	0.556867000
1	-2.334627000	-1.820224000	2.149401000
1	-2.943227000	-4.269671000	2.423348000
1	0.576282000	-6.384085000	-0.170576000
1	0.490297000	-5.629398000	-1.763093000
1	1.325779000	-5.017412000	1.850526000
1	1.759725000	-3.317710000	1.655695000
1	1.115408000	-3.170995000	-2.045725000
1	1.635294000	-2.225579000	-0.648883000
1	2.328498000	-4.616090000	-0.404739000
6	5.927116000	-1.588640000	-1.434198000
6	6.275512000	-2.892445000	-0.682812000
6	6.049228000	-2.660416000	0.827429000
6	4.469166000	-1.186513000	-1.166552000
6	5.206145000	0.155585000	0.819376000
6	4.591422000	-2.259556000	1.097746000
6	4.263258000	-0.960654000	0.341304000
6	7.733308000	-3.285598000	-0.947837000
6	8.353638000	-0.858538000	-1.214881000
6	8.688760000	-2.181752000	-0.476316000
6	8.475368000	-1.926963000	1.039675000
6	9.433619000	-0.817495000	1.518048000
6	9.085224000	0.486310000	0.766662000
6	9.311507000	0.254280000	-0.743579000
6	6.885367000	-0.479172000	-0.955825000
6	7.627437000	0.879465000	1.031687000
6	7.007098000	-1.547598000	1.298731000
6	6.671975000	-0.224383000	0.560166000
6	10.154600000	-2.561717000	-0.735526000

6	10.891570000	-1.219622000	1.250402000
6	10.769313000	-0.146580000	-1.013896000
6	11.097478000	-1.445481000	-0.257454000
1	6.075746000	-1.746207000	-2.511246000
1	5.607841000	-3.694021000	-1.026626000
1	6.285330000	-3.585761000	1.370517000
1	4.225371000	-0.271424000	-1.721336000
1	3.791422000	-1.971127000	-1.526505000
1	5.060854000	0.340561000	1.892282000
1	4.974866000	1.095248000	0.299765000
1	4.435746000	-2.117841000	2.174915000
1	3.915858000	-3.063257000	0.778072000
1	3.222653000	-0.672746000	0.533929000
1	7.971769000	-4.223306000	-0.427677000
1	7.885779000	-3.468613000	-2.020211000
1	8.494380000	-1.019165000	-2.294159000
1	8.703688000	-2.856299000	1.582497000
1	9.284989000	-0.659928000	2.595097000
1	9.752904000	1.287888000	1.110476000
1	9.075406000	1.179626000	-1.286666000
1	6.657048000	0.450163000	-1.498647000
1	7.388975000	1.817174000	0.511527000
1	7.474956000	1.062477000	2.104061000
1	6.866355000	-1.386971000	2.378009000
1	10.385869000	-3.501383000	-0.215915000
1	10.299881000	-2.746697000	-1.808432000
1	11.135364000	-2.134711000	1.805186000
1	11.569313000	-0.435008000	1.610355000
1	10.924999000	-0.288292000	-2.091064000
1	11.444878000	0.657121000	-0.694222000
1	12.138083000	-1.733389000	-0.450078000

#### Type B (-5°) on Cu(111)

6	5.721229000	1.595090000	1.017937000
6	6.157353000	2.874354000	0.270176000
6	6.162790000	2.575627000	-1.245278000
6	4.326096000	1.150213000	0.554637000
6	5.372360000	-0.255608000	-1.239036000
6	4.768178000	2.131909000	-1.711251000
6	4.351217000	0.858199000	-0.955707000
6	7.552862000	3.310157000	0.731256000
6	8.164479000	0.910389000	1.193640000
6	8.585258000	2.209275000	0.455723000
6	8.604660000	1.887861000	-1.062499000
6	9.640928000	0.781145000	-1.344140000
6	9.204804000	-0.498119000	-0.596380000
6	9.199366000	-0.199392000	0.919075000
6	6.757496000	0.488374000	0.736295000
6	7.809295000	-0.933922000	-1.057460000
6	7.197677000	1.465847000	-1.519844000

6	6.776898000	0.166960000	-0.781927000
6	9.989796000	2.631843000	0.912832000
6	11.036061000	1.226023000	-0.880841000
6	10.593978000	0.244326000	1.385048000
6	11.010939000	1.518036000	0.629503000
1	5.704872000	1.799951000	2.097157000
1	5.433300000	3.674414000	0.475537000
1	6.462749000	3.482906000	-1.787332000
1	4.016621000	0.253490000	1.106654000
1	3.589944000	1.933768000	0.775190000
1	5.391830000	-0.487606000	-2.312465000
1	5.080906000	-1.178048000	-0.718830000
1	4.777328000	1.942725000	-2.792332000
1	4.039891000	2.932927000	-1.531006000
1	3.355701000	0.539713000	-1.287920000
1	7.851535000	4.230779000	0.211662000
1	7.540608000	3.540329000	1.805314000
1	8.139941000	1.118224000	2.273758000
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