

**Size and branching effects on the fluorescence of benzylic dendrimers possessing one apigenin fluorophore at the core**

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ABSTRACT. Different generations of dendrimers incorporating one fluorescent core of apigenin and three Fréchet benzylic dendrons have been prepared. The chief geometric features of these dendrimers have been obtained by Molecular Dynamics simulations. These computational data suggest that the asphericities of dendrimers belonging to the third and fourth generations are considerably larger than those associated with lower radii of gyration. Fluorescence spectra of high generation dendrimers evolve along time and quantum yields show an appreciable lowering for the fourth generation dendrimer. All these data suggest aggregation phenomena and lower quantum yields for nonspheric dendrimers in solution.

## 1. Introduction

Since the discovery in 1978 of “cascade molecules” by Vögtle et al.,<sup>1</sup> dendrimers (as termed by Tomalia<sup>2</sup>) have emerged as a very important class of macromolecules with well-defined architectures. The nature of the cores, the different spacers and end groups, as well as the degrees of branching can be chosen among many different building blocks,<sup>3</sup> thus giving rise to a plethora of different families of dendrimers<sup>4</sup> with many applications in, among other fields, catalysis,<sup>5</sup> materials science,<sup>6</sup> supramolecular chemistry<sup>7</sup> and biomedicine.<sup>8</sup>

The structure and shape of dendrimers are difficult to determine and actually the usual analytical techniques<sup>9</sup> are pushed to their limits to characterize the identity, purity and structural elucidation of these macromolecules. In this respect, computational methods are very useful to describe adequately both the geometrical and dynamic behaviour of dendritic molecules.<sup>10</sup> Pioneering studies proposed that dendrimers in general exhibit density profiles in which a global minimum is located at the center, with a monotonic increase towards the periphery.<sup>11</sup> However, this general model was refined<sup>12</sup> and now it is generally admitted that this density profile is more complex, thus resulting in dense core regions and relatively less dense peripheries.

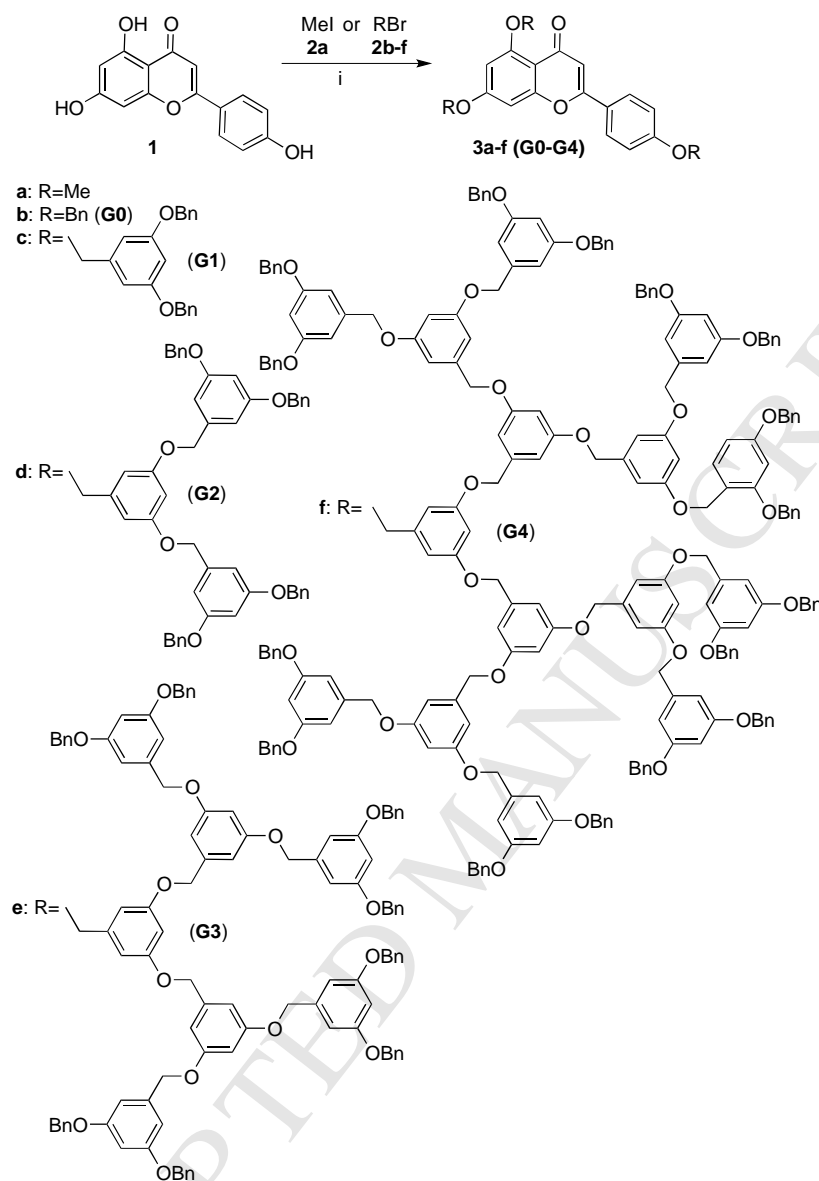
Fluorescent dendrimers<sup>13</sup> are particularly interesting because of their potential as analytical tools<sup>14</sup> or in light-harvesting devices,<sup>15</sup> organic light emitting diodes<sup>16</sup> (OLEDs), solar cells<sup>17</sup> or displays.<sup>18</sup> The chosen fluorophores can be installed at different parts of the macromolecule. In most cases, diverse fluorophores and/or donor/acceptor systems can be incorporated within the different branches or at the periphery. In these cases, however, the structure optical response relationship is difficult to rationalize. In previous work on dendrimers carried out in our group, we have analyzed the catalytic activity of dendrimers with one active site at the core. In this case a rationale of the catalytic activity of different

dendrimers possessing Fréchet dendrons was developed.<sup>19</sup> Following this approach, in this paper we would like to present a simple model describing the structure activity quantitative relationship of fluorescent dendrimers incorporating only one fluorophore at the core. As a case study, we have chosen apigenin,<sup>20</sup> a weak blue light emitting fluorophore that possesses three phenol groups amenable to Williamson coupling reactions with different Fréchet dendron bromides. The interplay between the *4H*-chromen-4-one fluorophore and the phenyl chromophores of the branches and at the periphery should result in different photophysical responses for the successive generations of dendrimers. As we will see, this design has permitted to find a simple model that connects the quantum yield of the fluorescent emission with an easy to compute and intuitive combined geometrical parameter.

## 2. Results and discussion

### 2.1. Preparation of apigenin derivatives.

We prepared compounds **3a-f** by Williamson reaction between **1** and halides **2a-f** in the presence of different bases (Scheme 1). The chemical yields of purified products were relatively low (15-40 %, see the Experimental Section) but satisfactory enough for our purposes.



**Scheme 1.** Synthesis of ethers **3a-f (G0-G4)** from apigenin **1**. Reagents and conditions: *i*: NaH (for **G0,G1**) or  $K_2CO_3$  (for **G2-G4**), 18-crown-6 (for **G2-G4**), r. t. (for **G0,G1**) or 80 °C (for **G2-G4**). Bn= Benzyl.

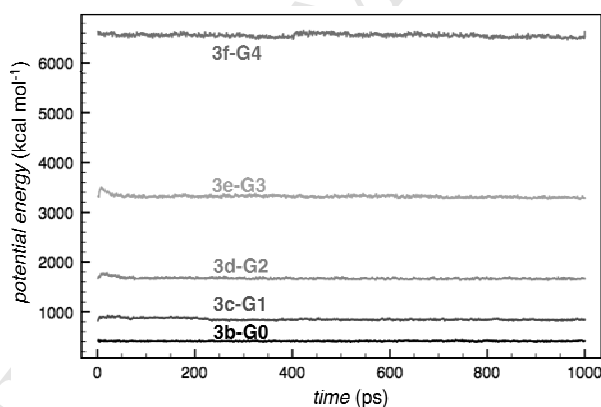
The reaction conditions reflect the increasing difficulty to accomplish the formation of the three C-O bonds along the different dendritic generations. Thus, formation of small compounds **3a-3c** (Apigenin derivatives **3b,c** being the zeroth and first-generation **G0** and **G1** in the dendrimer series) required NaH as a base and 20 hours at room temperature. In the case



of dendrimers **3d-f**, Williamson couplings involving Fréchet dendrons **2d-f** required potassium carbonate, 18-crown-6 as a cryptand of potassium and heating at 80 °C.

## 2.2. Molecular simulations and structural parameters of dendrimers **3b-f**.

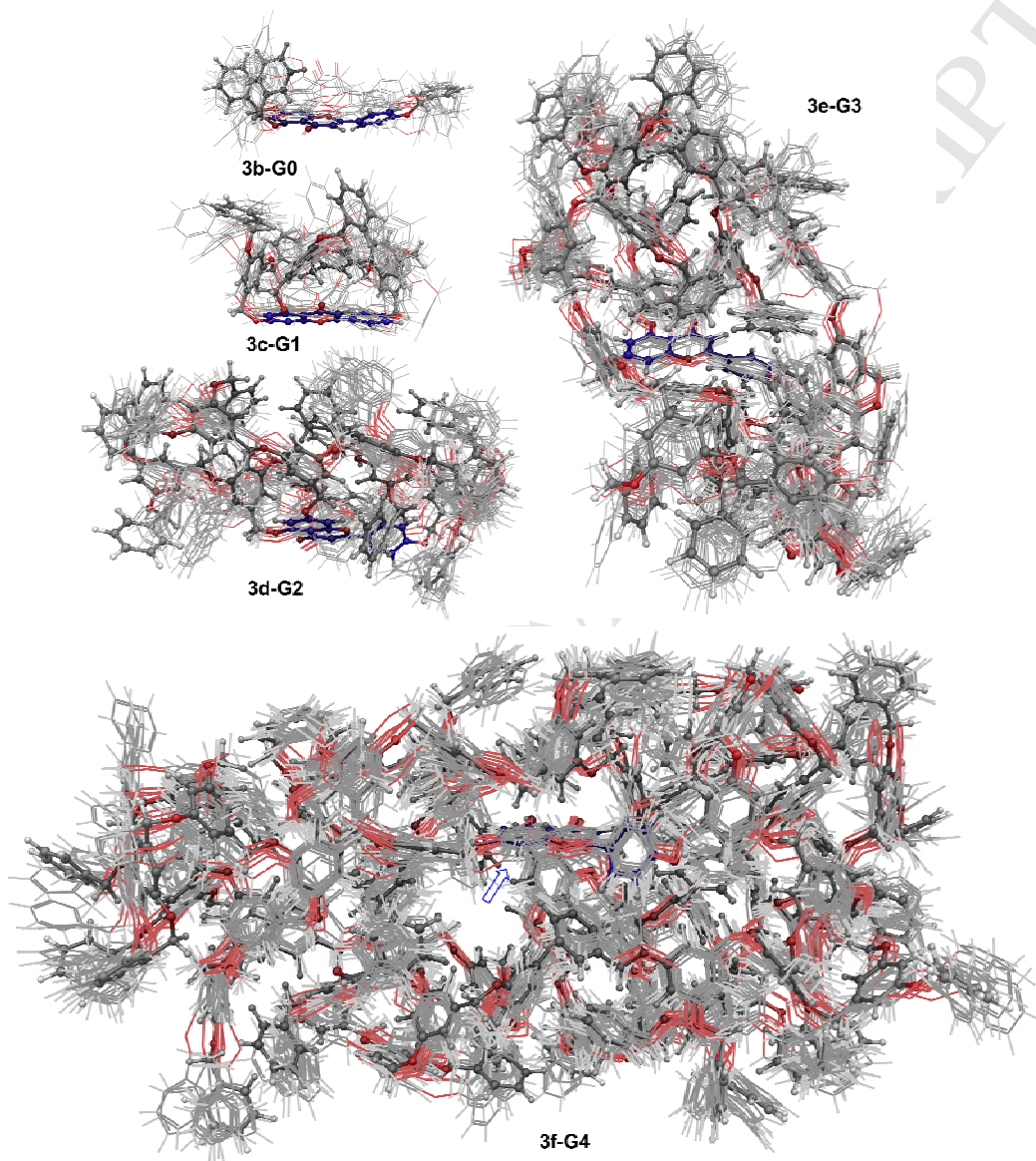
In order to gain a better understanding of the structural properties of compounds **3b-f** and their relationship with the observed properties (*vide infra*), we performed atomistic molecular dynamics (MD) simulations on these compounds using the MM3 force field.<sup>21</sup> Evolution of dendrimers **3b-f (G0-G4)** was simulated along 1000 ps. During the production time of the MD simulations, the fluctuating energy values were observed to be stable within the thermal limits (the relative root mean squared fluctuation in the energy ranged from 0.01 for the smallest system to 0.001 for the largest system), as it can be seen by inspection of the energy profiles gathered in Figure 1.



**Figure 1.** MM3 potential energy profiles for dendrimers **3b-f (G0-G4)** along the MD simulations.

The general shape of compounds **3b-G0** and dendrimers **3c-f (G1-G4)** can be appreciated in Figure 2, in which we have superimposed the ten most stable geometries obtained during the production time of the respective MD simulations. From these data it can be readily seen that lower dendrimers **3b-G0**, **3c-G1** and **3d-G2** permit contacts between the

apigenin and the external medium, whereas in higher dendrimers **3e-G3** and **3f-G4** these contacts are much more difficult.



**Figure 2.** Snapshots from the MD simulations of dendrimers **3b-G0**, **3c-G1**, **3d-G2**, **3e-G3** and **3f-G4**. The apigenin core in each dendrimer is highlighted in blue. The most stable structures are gathered in ball & stick representation. The remaining structures correspond to the 10 most stable structures within the 1000 ps simulation time. The hollow arrow in **3f-G4** indicates the position of the apigenin core.

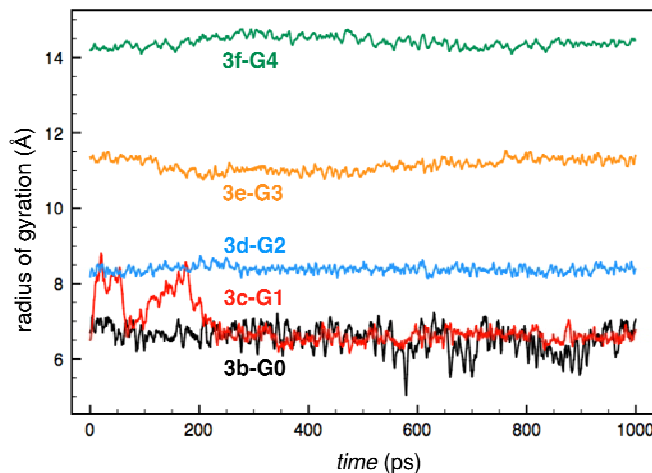
In order to quantify these geometric differences, we computed the radii of gyration for all the points generated along the MD simulations. The radius of gyration  $R_g$  is given by the following expression:

$$R_g = \left[ \frac{\sum_{i=1}^n m_i (\vec{r}_i - \vec{g})(\vec{r}_i - \vec{g})}{\sum_{i=1}^n m_i} \right]^{1/2} \quad (1)$$

where  $m_i$  is the mass of atom  $i$  ( $i=1,2,\dots,n$ ),  $\vec{r}_i$  is its position vector, and  $\vec{g}$  is the position vector of the center of masses:

$$\vec{g} = \frac{\sum_{i=1}^n m_i \vec{r}_i}{\sum_{i=1}^n m_i} \quad (2)$$

The fluctuation of the  $R_g$  values along the MD simulations for the different generations **G0-G4** are gathered in Figure 3 and the average values are reported in Table 1. Our results indicate that the  $R_g$  values of **3b-G0** and **3c-G1** are similar during most of the production time. The values obtained for **3d-G2** are slightly higher. Dendrimers **3e-G3** and **3f-G4** exhibit consistently larger radii of gyration and lower fluctuations, which indicate more rigid structures and larger atom densities at the respective cores and peripheries.



**Figure 3.** Evolution of the radius of gyration of dendrimers **3b-f (G0-G4)** along the production time of MD simulations.

The square of  $R_g$  is equal to the trace of the gyration tensor  $S$  of a given molecule and it is defined by eq 3.:

$$S = \frac{1}{M} \begin{pmatrix} \sum_i m_i (x_i - x_{cm})(x_i - x_{cm}) & \sum_i m_i (x_i - x_{cm})(y_i - y_{cm}) & \sum_i m_i (x_i - x_{cm})(z_i - z_{cm}) \\ \sum_i m_i (y_i - y_{cm})(x_i - x_{cm}) & \sum_i m_i (y_i - y_{cm})(y_i - y_{cm}) & \sum_i m_i (y_i - y_{cm})(z_i - z_{cm}) \\ \sum_i m_i (z_i - z_{cm})(x_i - x_{cm}) & \sum_i m_i (z_i - z_{cm})(y_i - y_{cm}) & \sum_i m_i (z_i - z_{cm})(z_i - z_{cm}) \end{pmatrix} \quad (3)$$

$$tr(S) = R_g^2 = tr \begin{pmatrix} L_1^2 & 0 & 0 \\ 0 & L_2^2 & 0 \\ 0 & 0 & L_3^2 \end{pmatrix} \quad (4)$$

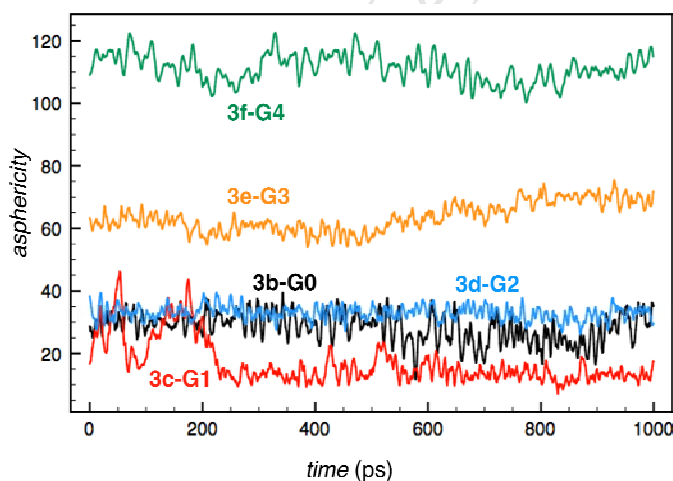
In the last term of Eq. 4 the tensor  $S$  is diagonalized such that the components  $L_i$  ( $i=1,2,3$ ) of  $R_g$  with respect to the corresponding main axes are assigned according to the following criterion:

$$L_1^2 > L_2^2 > L_3^2 \quad (5)$$

These  $L_i$  values can be used to quantify the shape of the molecule being considered. Thus, the asphericity  $a_s$  of one given molecular geometry is defined as<sup>22</sup>

$$a_s = L_1^2 - \frac{1}{2}(L_2^2 + L_3^2) \quad (6)$$

According to eq. 6,  $a_s$  reflects the anisotropy of the molecule with respect to the principal axes. For a perfect sphere, the magnitudes of the three main radii are identical ( $L_1 = L_2 = L_3$ ) and therefore  $a_s=0$ . In our case, values of  $a_s >0$  reflect the increasing anisotropy of dendrimers **3b-f** by departure from perfect sphericity. The average values of  $L_i$  and  $a_s$  are gathered in Table 1.



**Figure 4.** Evolution of the asphericity of dendrimers **3b-f (G0-G4)** along the production time of MD simulations.

**Table 1.** Average values<sup>[a]</sup> of radius of gyration ( $\langle R_g \rangle$ , in Å), its components along the main axes  $L_1$ - $L_3$  (in Å) and asphericities ( $\langle a_s \rangle$ , in Å<sup>2</sup>) of dendrimers **3b-f (G0-G4)**.

Dendrimer	$\langle R_g \rangle$	$\langle L_1 \rangle$	$\langle L_2 \rangle$	$\langle L_3 \rangle$	$\langle a_s \rangle$
<b>3b-G0</b>	6.07 ±0.07	5.59 ±0.26	2.07 ±0.05	1.20 ±0.15	28.30 ±1.42
<b>3c-G1</b>	6.53 ±0.02	5.05 ±0.79	3.52 ±0.06	2.23 ±0.10	16.84 ±1.07
<b>3d-G2</b>	8.36 ±0.01	6.75 ±0.10	4.20 ±0.10	2.74 ±0.78	32.94 ±0.34
<b>3e-G3</b>	11.21 ±0.12	9.15 ±0.17	5.16 ±0.10	3.66 ±0.05	63.73 ±0.50
<b>3f-G4</b>	14.82 ±0.16	12.29 ±0.46	6.85 ±0.40	4.83 ±0.08	116.05 ±1.23

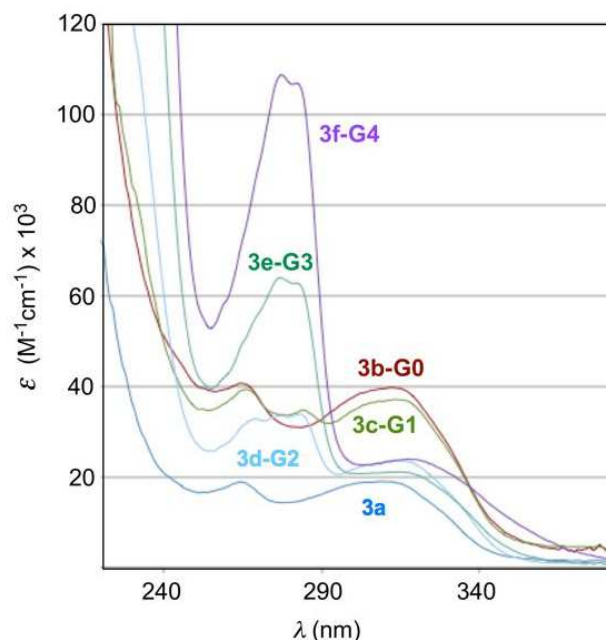
<sup>[a]</sup>All values correspond to the average values obtained along the MD simulations using the MM3 force field and eqs. 1-5.

Our computed values for asphericity show closely related values for **G0** and **G2**. First generation dendrimer **G1** is more spheric than apigenine derivatives **G0** and **G2**, **G3** showing a somewhat larger value of about 64 Å<sup>2</sup>. However, the largest asphericity value was computed for **G4**, with a value of  $a_s$  almost twice than that obtained for **G3** (See Figure 4 and Table 1). This suggests that the hydrodynamic behaviour of **G4** is determined by a larger departure from sphericity and aggregation phenomena to form more isotropic structures with lower  $a_s$  values should be expected.<sup>23</sup>

### 2.3. Photophysics of compounds 3a-f.

Absorption spectra of compounds **3a-f** show two zones which provide different structural information (Figure 5). One of them, associated with a maximum near 315 nm, is related to the fluorophore core. The other zone, with a maximum absorption near 280 nm, may provide some information on the fluorescence generated by the benzylic dendrons. In all cases, we observed that absorbances at both 280 and 315 nm increase linearly with concentration. Inspection of Figure 5 shows quite similar UV spectra for **G0-G2**, with a distinctive profile for **G4**, **G3** being between both subsets. This can be explained in terms of a effect of the medium. According to Toptygin<sup>24</sup> the extinction coefficient as well as the radiative decay rate

depend on the refractive index. In spite of the fact that the increase with the refractive index is higher for the radiative decay rate, it also occurs for the extinction coefficient and it was observed for the first generations of dendrimers.



**Figure 5.** Absorption spectra of compounds **3a-f** in THF.

Quantum yields were measured at the previously described two excitation wavelengths. Apigenin exhibits double fluorescent emission in methanol, with two maxima at 430 nm and 534 nm.<sup>25</sup> When excitation is done at 300 nm, emission shows a maximum at 430, and a shoulder at 534 nm. By exciting at 357 nm, only emission at 534 nm is obtained. The emission spectra of the dendrimers when exciting at 280 nm are similar than those when exciting at 315 nm (see Supplementary data for further information). This has been reported<sup>26</sup> to be due to an intramolecular proton transfer between a phenolic OH (in C-5) and the oxygen of carbonyl (in C-4). In the case of **3a**, the latter emission is not present since the phenolic OH has been methoxylated and, therefore, there is no possibility for an intramolecular proton

transfer. As a consequence, the quantum yield of **3a** ( $1.7 \times 10^{-3}$ , see Table 2) is higher than that of apigenin ( $4 \times 10^{-4}$ ).

**Table 2.** Photophysical data of apigenin derivatives **3a-f**.

Dendrimer	$\Phi$ <sup>[a]</sup> ( $\lambda_{exc}$ = 315 nm)	$\Phi$ <sup>[a]</sup> ( $\lambda_{exc}$ = 280 nm)	$\tau$ (ns) <sup>[b]</sup>	$k_r \times 10^{-9} (\text{s}^{-1})$ <sup>[c]</sup>	$k_{nr} \times 10^{-9} (\text{s}^{-1})$ <sup>[d]</sup>
<b>3a</b>	0.0017	0.0018	0.88	0.001924	1.129810
<b>3b-G0</b>	0.0053	0.0045	0.82	0.006498	1.219443
<b>3c-G1</b>	0.0095	0.0055	0.86	0.011017	1.148672
<b>3d-G2</b>	0.0112	0.0039	0.86	0.012984	1.146302
<b>3e-G3</b>	0.0033	0.0021	1.03	0.003219	0.972390
<b>3f-G4</b>	0.0077	0.0017	0.75	0.010216	1.316572

<sup>[a]</sup> Quantum yields measured in THF at different excitation wavelengths using quinine sulphate as standard (See the Experimental Section). <sup>[b]</sup> Time-domain excited state lifetime. <sup>[c]</sup> Radiative constants. <sup>[d]</sup> Non-radiative constants, measured in THF.

Quantum yields and radiative constants  $k_r$  of dendrimers were found to be higher than those of **3a**, and increase on going from **3b-G0** to **3d-G2** at  $\lambda_{exc}=315$  nm. However, from this latter dendrimer these values decrease to achieve a quantum yield of **3f-G4** at 280 nm similar to that of **3a**. In the case of  $\lambda_{exc}=280$  nm, **3c-G1** showed the highest quantum yield and a monotonous decrease was observed on going from **G2** to **G4**. The observed enhancements of fluorescence can be related to the contribution of the refractive index, according to the Toptygin equation<sup>24</sup>:

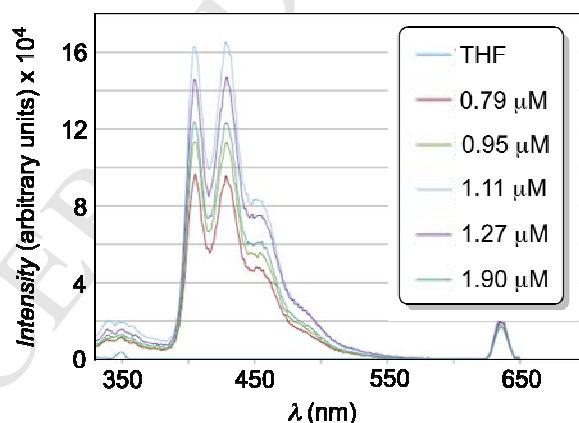
$$k_r = nf^2 k_{r0} \quad (7)$$

where  $n$  is the refractive index of the host medium;  $f$  is a function of  $n$ , and depends on the geometry of the local environment, and  $k_{r0}$  is the radiative decay constant in vacuum. In the case of **3a**,  $n$  is that of solvent. In the case of dendrimers **G0-G4**, the  $n$  value associated with the local medium that would correspond to that of the aromatic dendrons in the



microenvironment of the fluorophore. It is reasonable to think that, at least for dendrimers **G0-G2**, it will be higher than that of the solvent. Likewise, it should become higher with the degree of branching. However, our results also suggest that from a certain degree of branching on, aggregations of dendrimers occur in THF. This should lead to a decrease of the fluorescent emission, as it can be seen by inspection of the quantum yields reported in Table 1.

Emission spectra of higher dendrimers were found to evolve over time, which also suggests aggregation phenomena. Figure 6 shows the spectra of solutions of different concentrations of **3e-G3** 48 hours after their preparation, showing that these spectra and the corresponding aggregates become stable after sufficient time. These data are consistent with the structural results obtained from the MD simulations: the lower asphericity shown by **G3** is, at least in part, responsible for these aggregation phenomena and, into a higher extension, those associated with **G4**.



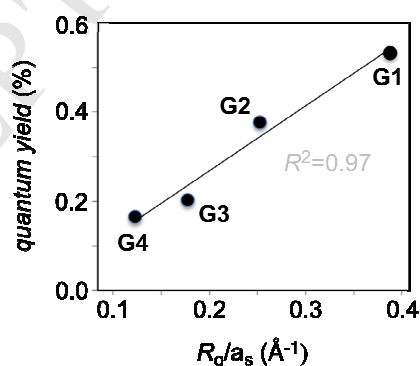
**Figure 6.** Emission spectra of **3e-G3** at five different concentrations and after 48 hours of their preparation.

From the data collected in Tables 1 and 2, the evolution of the quantum yields along the **G1-G4** series can be quantified. We have found a linear correlation between the

$\langle R_g \rangle / \langle a_s \rangle$  ratio and the quantum yield associated with the fluorescent emission with a wavelength of 280 nm, namely that associated with  $\pi \rightarrow \pi^*$  transitions involving the Fréchet dendrons of **G1-G4**. This correlation is given by the following expression:

$$\Phi = K_G \frac{\langle R_g \rangle}{\langle a_s \rangle} \quad (8)$$

with  $K_G=0.014 \text{ \AA}$  (Figure 7). Our attempts to find a similar correlation associated with the excitation of the apigenin fluorophore met with no success. These results suggest that the combined  $\langle R_g \rangle / \langle a_s \rangle$  parameter can be useful to design dendrimers with better photophysical properties by increasing the generation number (with larger radii of gyration) while keeping asphericities as low as possible. Note however, that the relation in Eq. 8 is found to hold for dendrimers with shapes studied in this work which are characterized by relatively large value of asphericity. Further studies are needed in order to elucidate the behavior of dendrimers with smaller value of  $\langle a_s \rangle$  and, in particular, for perfectly spherical molecules ( $\langle a_s \rangle$ ) because then the right hand side of Eq. 8 diverges



**Figure 7.** Correlation between structural data of dendrimers **G1-G4** and quantum yields measured with an excitation wavelength of 280 nm.

### 3. Conclusions

In this paper we report the preparation and the main geometrical and photophysical properties of different dendrimers possessing an apigenin fluorophore at the core and different Fréchet dendrons. The coupling between the core and the dendrons has been carried out via Williamson reactions between the three phenolic groups of apigenin and the corresponding Fréchet bromides. A transition from nearly spherical to highly aspherical dendrimers has been detected on going from the first three generations to **G3** and, specially, **G4**. It is found that for lower generation dendrimers the quantum yields of the fluorescent emissions increase with the generation number or the radius of gyration as it could be expected for more isolated fluorophores. This maximum quantum yield is achieved for **G2**. However, there is a significant decay in the quantum yields of **G3** and **G4**, which parallels an increase in aspheredicity for these latter dendrimers. These data, together with the evolution of the emission spectra, indicate that aggregation phenomena are relevant in **G3** and **G4**, thus resulting in more efficient nonradiative decays and therefore in lower quantum yields. These results suggest that, in order to improve the quantum yields of fluorescent emission of dendrimers highly spheric low associative dendrimers should be designed.

## 4. Experimental section

### 4.1. Computational methods

All the computational studies reported in this paper were based upon molecular mechanics<sup>27</sup> (MM) and molecular dynamics (MD)<sup>28</sup>. In both, the MM3 method developed by Allinger et al. as implement in the *MacroModel*<sup>29</sup> package was used. All MD simulations were performed with SHAKE<sup>30</sup> to constrain the C-H bonds. The temperature was set up to 298 K. The system was equilibrated for 1 ns with time steps of 1 fs. This equilibration time is 10 times longer than the expected value for the relaxation time of dendrimers<sup>31</sup> of this size. The production run was started from this point and lasted another nanosecond with time steps of 1 fs. In all

cases, we observed that during the production period, the energy and temperature of the whole system were equilibrated. During the production run, the coordinates were saved each picosecond, which implies a total of 1000 structures. These structures were used to calculate the averages of the properties specified below. To calculate these properties, programs based on the DYNAMO library<sup>32</sup> were written.

#### 4.2. General experimental methods

Reagents and solvents were purchased from commercial suppliers and used without further purification. Fréchet-type dendrons of generation number one to four **2c** – **2f** were prepared according to procedure reported by Fréchet.<sup>33</sup> NaH was used in form of 60% (w/w) dispersion in mineral oil. Column chromatographies were carried out with silica gel 60 (0.040 – 0.063 mm). All melting points are uncorrected. NMR spectra were recorded in CDCl<sub>3</sub> and using frequencies as indicated bellow. Mass spectra were measured using electrospray ionisation at positive mode. MALDI-TOF MS spectra were measured using trihydroxyacetophenone in 60% acetonitrile with 0.1% of TFA as matrix. MALDI-TOF spectrum of dendrimer **3f** was recorded in linear mode using sinapic acid in 60% acetonitrile with 0.1% of TFA as matrix.

*5,7,4'-trimethoxyflavone*,<sup>34</sup> **3a**. To a solution of apigenin (50 mg, 0.19 mmol) in dry dimethylformamide (2 ml) was added NaH (20 mg, 0.5 mmol), under cooling by ice bath. After stirring for 10 minutes under argon, methyl iodide (0.15 ml, 2.56 mmol) was added dropwise. The reaction mixture was stirred for 20 hours at room temperature and then, it was diluted by dichloromethane, washed by water, organic phases collected and dried (MgSO<sub>4</sub>), and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (CH<sub>2</sub>Cl<sub>2</sub>/MeOH) and by precipitation by hexanes from ethyl acetate to yield title product as yellow solid (40%, 30 mg): IR 1640, 1601, 1573, 1511 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, 25 °C)  $\delta$  = 7.81 (d, *J* = 8.5 Hz, 2 H), 6.98 (d, *J* = 8.5 Hz, 2 H), 6.59 (s, 1 H), 6.54 (d, *J*

= 1.8 Hz, 1 H), 6.35 (d,  $J = 2.3$  Hz, 1 H), 3.94 (s, 3 H), 3.90 (s, 3 H), 3.87 (s, 3 H) ppm;  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta = 177.60, 163.88, 162.02, 160.89, 160.65, 159.82, 127.58$  (2C), 123.85, 114.33 (2C), 109.23, 107.69, 96.06, 92.81, 56.40, 55.71, 55.45 ppm. MS (ESI)  $m/z$ : found 312.9  $[\text{M}+\text{H}]^+$ ; calcd. 313.1.

*4',5,7-trisbenzyloxyflavone*,<sup>35</sup> **3b-G0**. To a solution of apigenin (40 mg, 0.15 mmol) in dry dimethylformamide (2 ml) was added NaH (20 mg, 0.5 mmol), under cooling by ice bath. After stirring for 10 minutes under argon, benzyl bromide (0.2 ml, 1.69 mmol) was added dropwise. The reaction mixture was stirred for 20 hours at room temperature and then, it was diluted by ethyl acetate, washed by water, organic phases collected and dried ( $\text{MgSO}_4$ ), and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (gradient of ethyl acetate in toluene/hexane (60/40 v/v)) and precipitated by hexanes from ethyl acetate to yield title product (25%, 21 mg) as slightly yellow solid: IR 1638, 1601, 1509, 1163  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta = 7.82$  (d,  $J = 8.5$  Hz, 2 H), 7.62 (d,  $J = 7.6$  Hz, 2 H), 7.28 - 7.49 (m, 13 H), 7.07 (d,  $J = 8.5$  Hz, 2 H), 6.64 (d,  $J = 2.1$  Hz, 1 H), 6.58 (s, 1 H), 6.49 (d,  $J = 1.8$  Hz, 1 H), 5.23 (s, 2 H), 5.14 (s, 2 H), 5.11 (s, 2 H) ppm;  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta = 177.32, 162.81, 161.17, 160.65, 160.54, 159.70, 136.44, 136.29, 135.73, 128.75, 128.74, 128.69, 128.55, 128.41, 128.21, 127.64, 127.59, 127.45, 126.58, 124.13, 115.23, 109.87, 107.82, 98.37, 94.28, 70.77, 70.47, 70.17$  ppm. MS (ESI)  $m/z$ : found 541.5  $[\text{M}+\text{H}]^+$ ; calcd. 541.6.

*Dendrimer 3c-G1*. To a solution of apigenin (19 mg, 0.070 mmol) in dry dimethylformamide (2 ml) was added NaH (15 mg, 0.38 mmol), under cooling by ice bath. The mixture was stirred for 10 minutes under argon and then, **2c** (150 mg, 0.39 mmol) was added. The reaction mixture was stirred for 20 hours at room temperature and then it was diluted by dichloromethane and washed by water. Organic phases were collected, dried ( $\text{MgSO}_4$ ), and evaporated under reduced pressure. The residue was purified by flash chromatography on

silica gel (gradient of ethyl acetate in toluene/hexane (60/40 v/v)) and precipitated two times by pentane from ethyl acetate to yield corresponding product (25%, 21 mg) as a colourless solid: mp 113-114 °C, IR 1640, 1592, 1145, 1049  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta$  = 7.81 (d,  $J$  = 8.8 Hz, 2 H), 7.28 - 7.47 (m, 30 H), 7.04 (d,  $J$  = 9.1 Hz, 2 H), 6.93 (d,  $J$  = 2.3 Hz, 2 H), 6.65 - 6.71 (m, 4 H), 6.62 (s, 1H), 6.52 - 6.62 (m, 4 H), 6.45 (d,  $J$  = 2.1 Hz, 1 H), 5.18 (s, 2H), 5.08 (s, 6H), 5.04 (s, 10H) ppm;  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta$  = 177.24, 162.63, 161.04, 160.56, 160.28, 160.25, 160.21, 159.64, 159.53, 139.01, 138.75, 138.13, 136.98, 136.69, 136.63, 128.59, 128.47, 128.05, 128.03, 127.84, 127.67, 127.63, 127.51, 127.50, 124.19, 115.25, 109.90, 107.84, 106.41, 106.32, 105.31, 101.81, 101.68, 101.61, 98.32, 94.37, 70.60, 70.26, 70.17, 70.15, 70.10, 70.02 ppm. MS (ESI)  $m/z$  found 1176.8  $[\text{M}+\text{H}^+]$ , calcd. 1176.44; Anal. Calcd. for  $\text{C}_{78}\text{H}_{64}\text{O}_{11}$ : C, 79.57 H, 5.48. Found: C, 79.78 H, 5.64.

**Dendrimer 3d-G2.** Apigenin (7.4 mg, 0.027 mmol) was dissolved in mixture of DMF and toluene (2 ml, 1/1 v/v). Then,  $\text{K}_2\text{CO}_3$  (75 mg, 0.54 mmol), 18-crown-6 (5 mg, 0.02 mmol) and **2d** (154 mg, 0.19 mmol) were added. The reaction mixture was stirred at 80 °C for 20 hours. Then, it was diluted by dichloromethane and washed by water. Organic phases were collected, dried ( $\text{MgSO}_4$ ), and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (gradient of diethyl ether in toluene/hexane (75/25 v/v)) and precipitated by pentane from THF to yield title product (40%, 28 mg) as a colourless solid glass: IR 1641, 1592, 1145, 1044  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta$  = 7.73 (d,  $J$  = 9.1 Hz, 2 H), 7.27 - 7.47 (m, 60 H), 7.00 (d,  $J$  = 9.1 Hz, 2 H), 6.93 (d,  $J$  = 2.1 Hz, 2 H), 6.62 - 6.74 (m, 15 H), 6.43 - 6.61 (m, 12 H), 6.47 (d,  $J$  = 2 Hz, 1 H), 5.15 (s, 2 H), 4.90 - 5.07 (m, 40 H) ppm;  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ , 25 °C)  $\delta$  = 177.18, 162.65, 161.01, 160.54, 160.18, 160.14, 160.08, 159.63, 159.52, 143.15, 139.47, 139.15, 139.07, 139.00, 138.74, 138.11, 136.85, 136.73, 136.72, 128.57, 128.51, 128.00, 127.99, 127.90, 127.61, 127.54, 127.51,

127.29, 124.14, 115.18, 109.86, 107.82, 106.47, 106.41, 106.39, 105.28, 101.83, 101.70, 101.59, 101.56, 70.12, 70.07, 70.01, 70.00 ppm. MS (MALDI-TOF)  $m/z$  found 2448.5  $[M+H]^+$ , calcd. 2449.9; found 2472.4  $[M+Na]^+$ , calcd. 2471.9; found 2488.5  $[M+K]^+$ , calcd. 2487.9; Anal. Calcd. for  $C_{162}H_{136}O_{23}$ : C, 79.39 H, 5.59. Found: C, 79.22 H, 5.47.

**Dendrimer 3e-G3.** Apigenin (6.1 mg, 0.023 mmol) was dissolved in mixture of DMF and toluene (2 ml, 1/1 v/v). Then,  $K_2CO_3$  (30 mg, 0.22 mmol), 18-crown-6 (5 mg, 0.019 mmol) and **2e** (150 mg, 0.091 mmol) were added. The reaction mixture was stirred at 80 °C for 20 hours. Then, it was diluted by dichloromethane and washed by water. Organic phases were collected, dried ( $MgSO_4$ ), and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (gradient of diethyl ether in toluene/hexane (75/25 v/v)) and precipitated two times by pentane from THF to yield title product (25%, 34 mg) as colourless solid glass: IR: 1641, 1592, 1147, 1044  $cm^{-1}$ ;  $^1H$  NMR (500 MHz,  $CDCl_3$ , 25 °C)  $\delta$  = 7.67 (d,  $J$  = 8.8 Hz, 2 H), 7.18 – 7.47 (m, 120 H), 6.93 (m, 4 H), 6.45 - 6.72 (m, 63 H), 6.41 (br. s., 1 H), 5.09 (br. s., 2 H), 4.78 - 5.04 (m, 88 H) ppm;  $^{13}C$  NMR (126 MHz,  $CDCl_3$ , 25 °C)  $\delta$  = 160.14, 160.12, 160.08, 160.06, 160.04, 159.96, 139.48, 139.28, 139.17, 136.79, 136.74, 128.55, 128.54, 128.51, 127.96, 127.93, 127.91, 127.52, 127.51, 106.42, 106.36, 101.70, 101.63, 101.57, 101.54, 70.10, 70.06, 70.03, 69.96, 69.93 ppm. MS (MALDI-TOF)  $m/z$  found 4996.4  $[M+H]^+$ , calcd. 4995.9; found 5019.5  $[M+Na]^+$ , calcd. 5018.0. Anal. Calcd. for  $C_{330}H_{280}O_{47}$ : C, 79.31 H, 5.65. Found: C, 79.46 H, 5.78.

**Dendrimer 3f-G4.** Apigenin (1.6 mg, 0.0059 mmol) was dissolved in mixture of DMF and toluene (1 ml, 1/1 v/v). Then,  $K_2CO_3$  (15 mg, 0.11 mmol), 18-crown-6 (3 mg, 0.011 mmol) and **2f** (70 mg, 0.0208 mmol) were added. The reaction mixture was stirred at 80 °C for 20 hours. Then, it was diluted by dichloromethane and washed by water. Organic phases were collected, dried ( $MgSO_4$ ), and evaporated under reduced pressure. The residue was purified by flash chromatography on silica gel (gradient of diethyl ether in toluene/hexane (75/25 v/v))

and precipitated by pentane from THF to yield title product (15%, 9 mg) as a colourless solid glass: IR: 1641 (small intensity), 1590, 1142, 1040  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )  $\delta$  = 7.63 (d,  $J$  = 8.8 Hz, 2 H), 7.19 - 7.37 (m, 240 H), 6.88 (d,  $J$  = 8.8 Hz, 2 H), 6.80 (m, 2 H), 6.70 (br. s., 2 H), 6.54 - 6.66 (m, 78 H), 6.43 - 6.54 (m, 53 H), 6.33 (d,  $J$  = 8.8 Hz, 1 H), 4.77 - 4.98 (m, 186 H) ppm;  $^{13}\text{C}$  NMR (200 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )  $\delta$  = 160.13, 160.11, 160.09, 160.07, 160.05, 160.02, 160.00, 159.94, 139.24, 139.19, 139.17, 136.76, 136.74, 136.73, 128.53, 128.51, 128.50, 127.94, 127.91, 127.89, 127.51, 106.39, 106.35, 106.33, 101.56, 101.54, 101.53, 101.49, 101.47, 70.02, 70.00, 69.96, 69.91, 69.89, 69.88, 69.84 ppm. MS (MALDI-TOF)  $m/z$  found 10121  $[\text{M}+\text{H}]^+$  calcd. 10092.

### 4.3. Spectroscopic measurements

UV/vis absorption and photoluminescence measurements were carried out on an absorption spectrometer (Shimadzu UV-2401-PC) and a fluorescence spectrophotometer (FLUOROMAX-P, Jobin Yvon), respectively at ambient conditions, using standard 10 mm cells and THF as solvent.

Fluorescence quantum yields of each compound ( $\Phi_x$ ) were determined by the method described by Williams et al.,<sup>36</sup> using quinine sulphate (in 0.1M  $\text{H}_2\text{SO}_4$ ) as standard which has a known fluorescence quantum yield ( $\Phi_{\text{ST}} = 0.54$ ), according to

$$\phi_X = \phi_{ST} \frac{Grad_X}{Grad_{ST}} \frac{\eta_X^2}{\eta_{ST}^2}$$

Where *Grad* is the slope from the plot of integrated fluorescence intensity vs absorbance at the same excitation wavelength, and  $\eta$  stands for the refractive index of the solvent (1.3332 for sulphuric acid solution of quinine, and 1.407 for THF).



Absorbances of five concentrations of the standard (in H<sub>2</sub>SO<sub>4</sub>) and each sample (in THF) were measured. Concentrations have been chosen which provide absorbances lower than 0.1 at and above the excitation wavelength, to avoid inner filter effects.

Wavelength at which the standard and samples absorb (either 315 nm or 280 nm) was chosen as excitation wavelength. Emission spectra were recorded on the same solutions under constant conditions, 48 hours after stabilization (slit width: 10 nm).

ORIGIN 8.0 was used for integrating the area of emission spectra. Residual fluorescence of solvents has been corrected. Five-point Area-Absorbance regressions were plotted for the standard and each compound.

Time-domain excited-state lifetimes were measured using an IBH 5000F coaxial nanosecond flashlamp, in a FL3-11 Fluorolog equipment.

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### **Supplementary data**

Scanned photocopies of  $^1\text{H}$  and  $^{13}\text{C}$  NMR data and MD input files (*Maestro-Macro Model* format) were supported. Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.tet.x>

## References and Notes

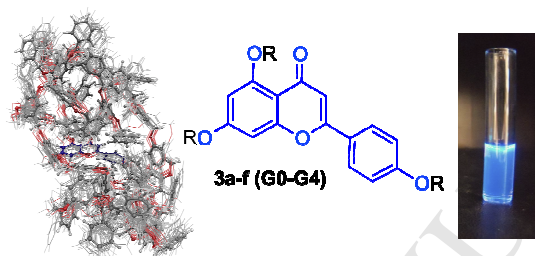
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## Graphical Abstract



## Size and Branching Effects on the Fluorescence of Benzylic Dendrimers Possessing One Apigenin Fluorophore at the Core

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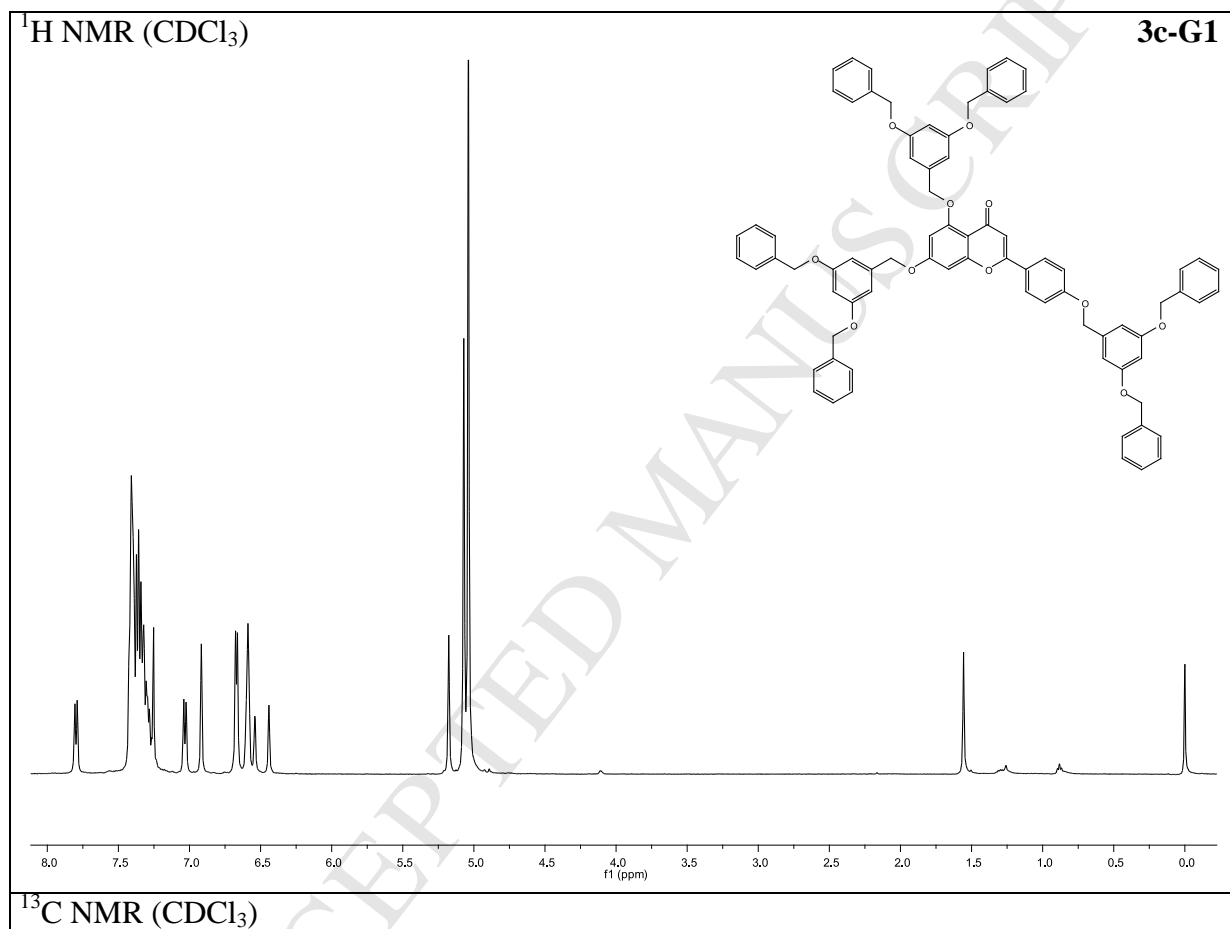
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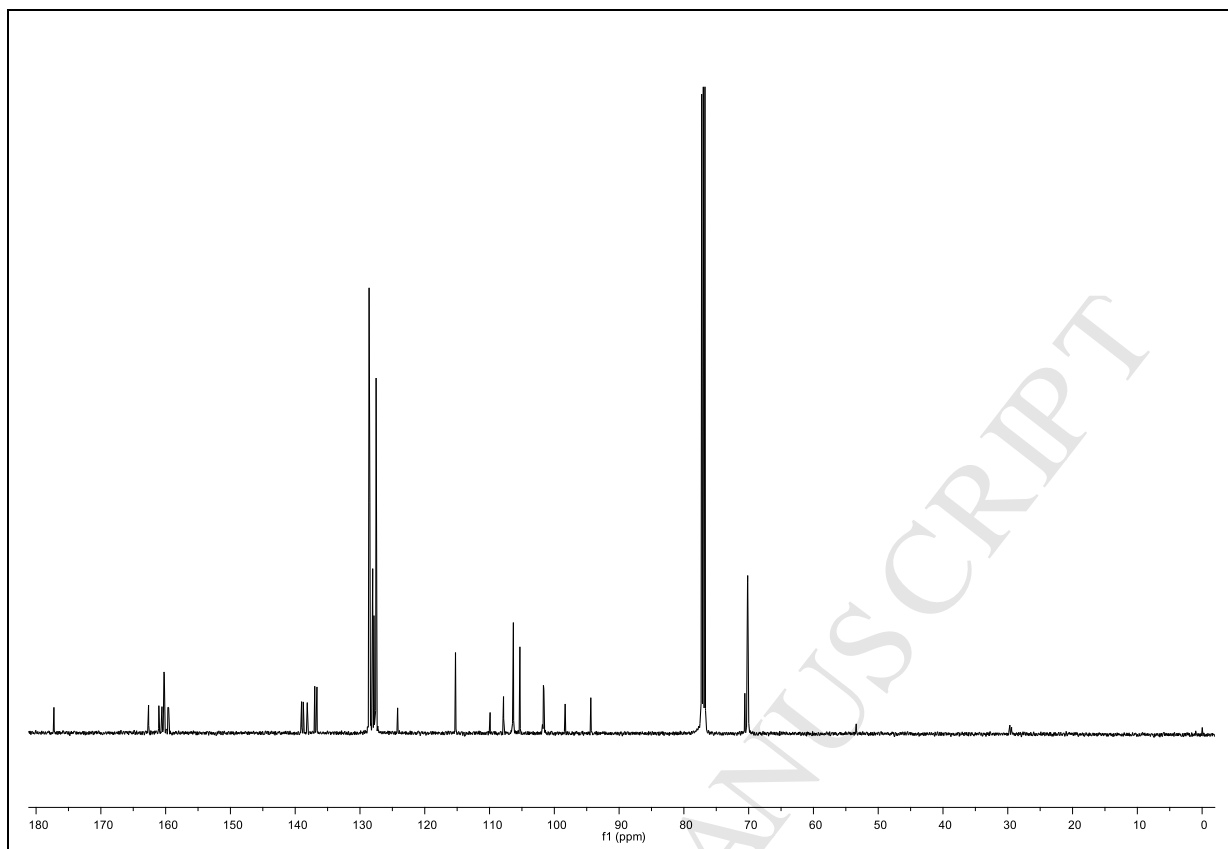
### Supplementary Data

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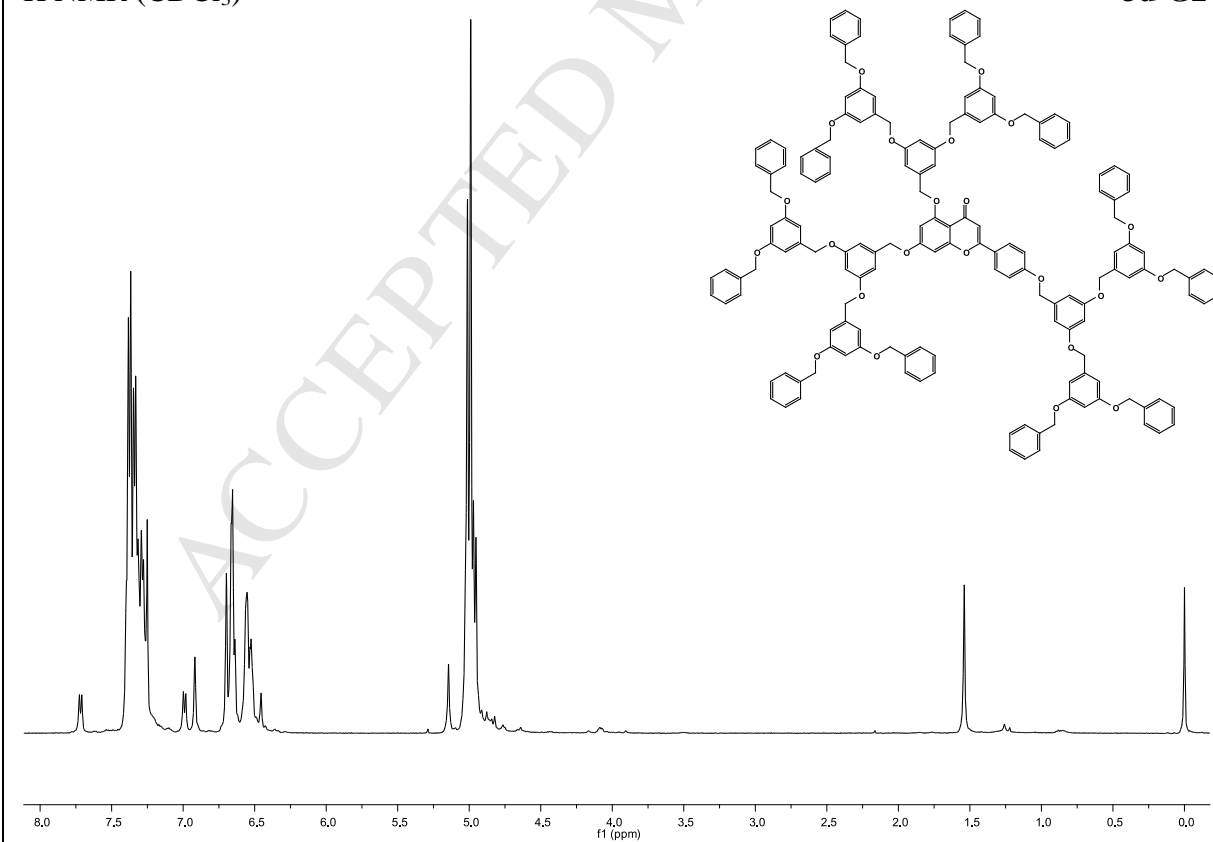
Item	Page(s)
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of new compounds	S2-S6
UV-vis spectra of compounds	S7-S9
Fluorescence spectra of compounds	S10-S13
Relative RMDS for all the system	S14
Starting geometries of dendrimers 3b-f (G0-G4)	S15-S53

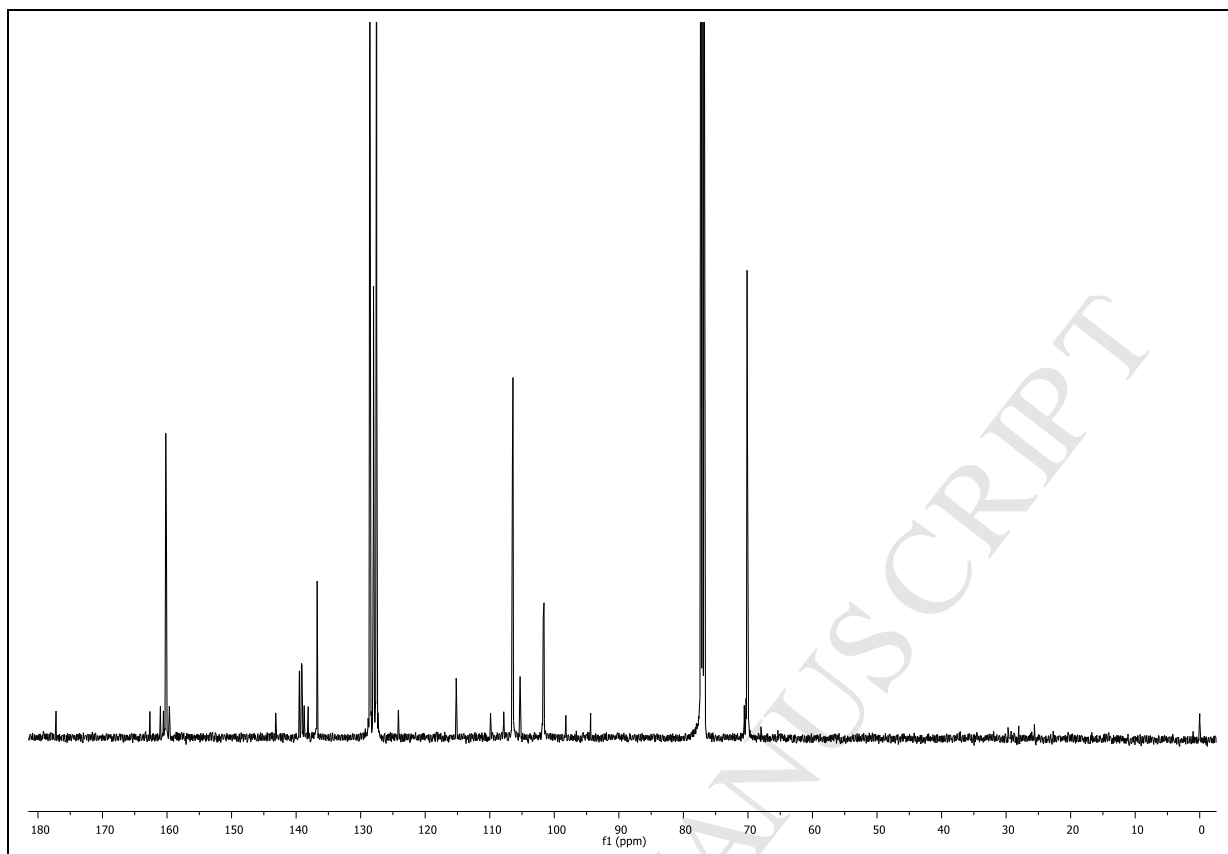
**$^1\text{H}$  NMR AND  $^{13}\text{C}$  NMR SPECTRA OF NEW COMPOUNDS**



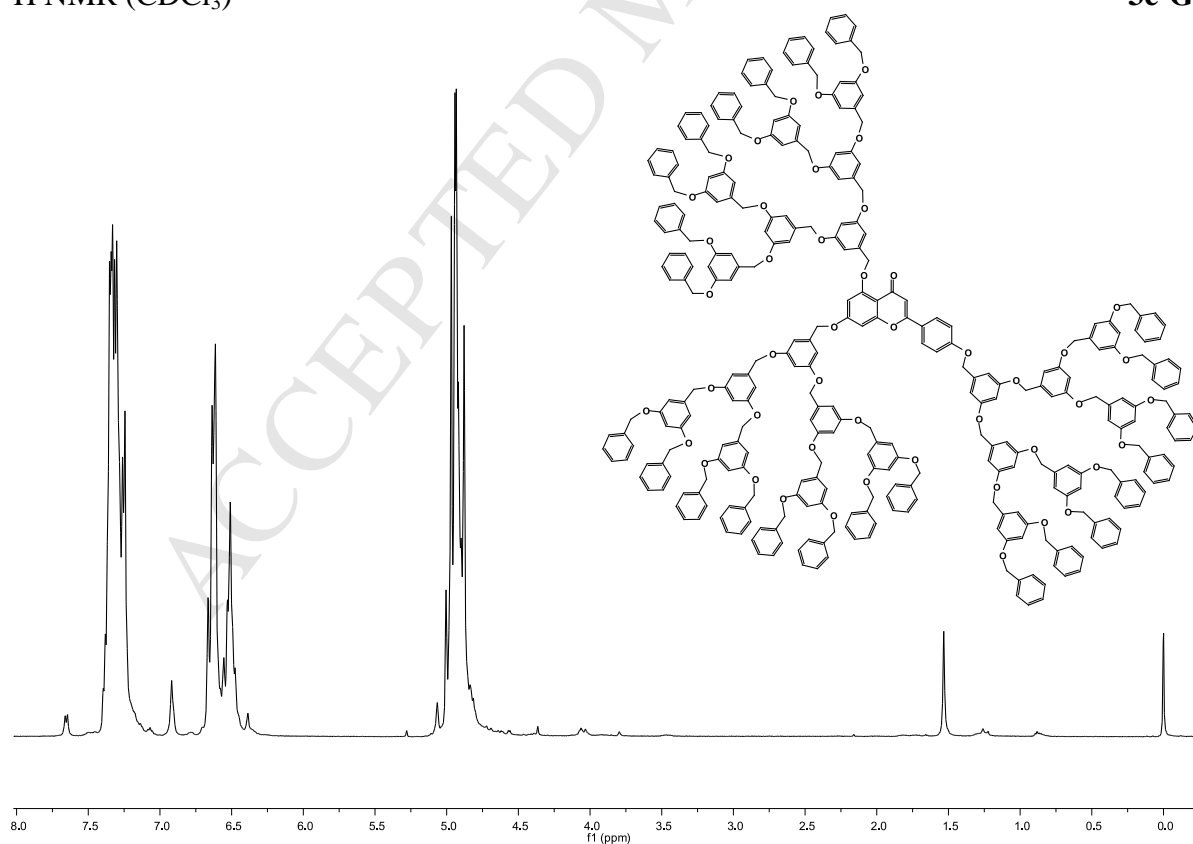
 $^1\text{H}$  NMR (CDCl<sub>3</sub>)

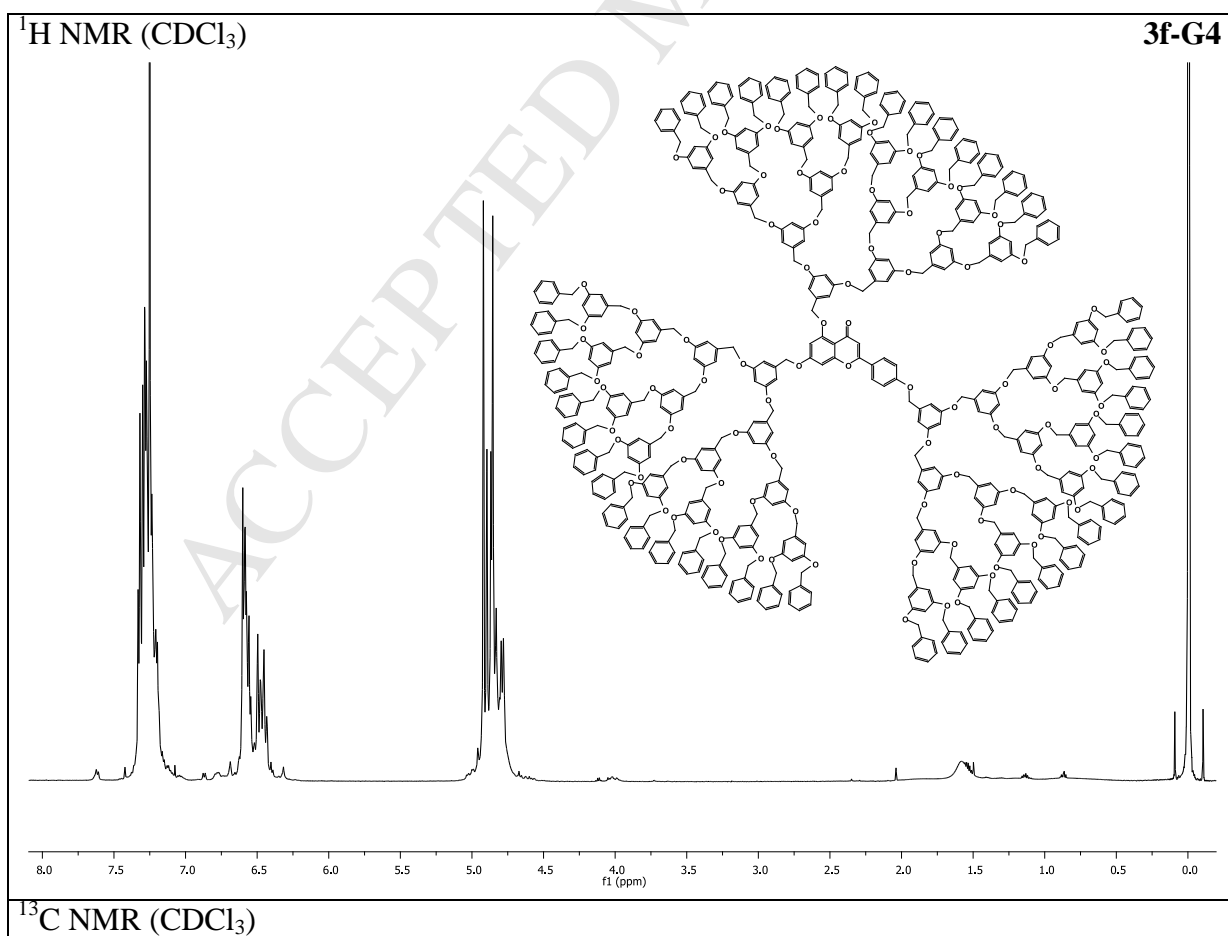
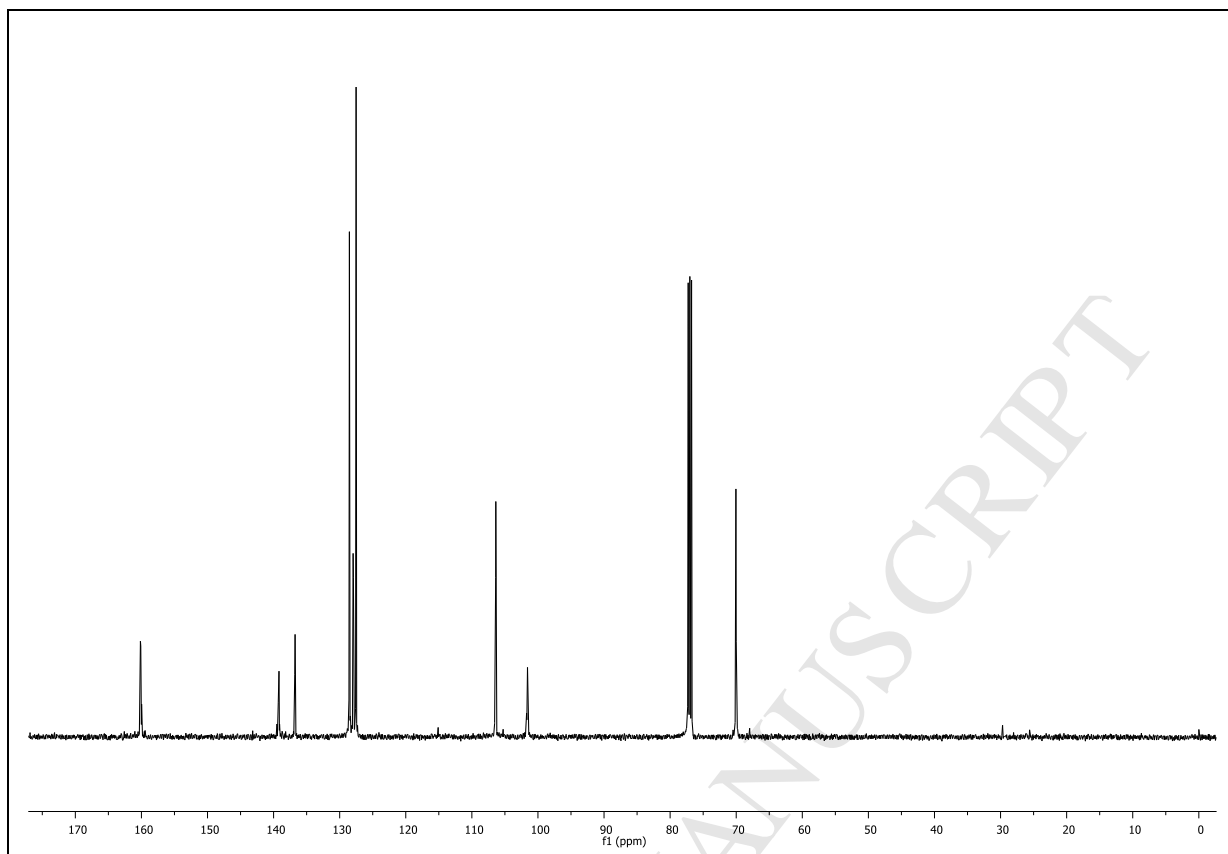
3d-G2

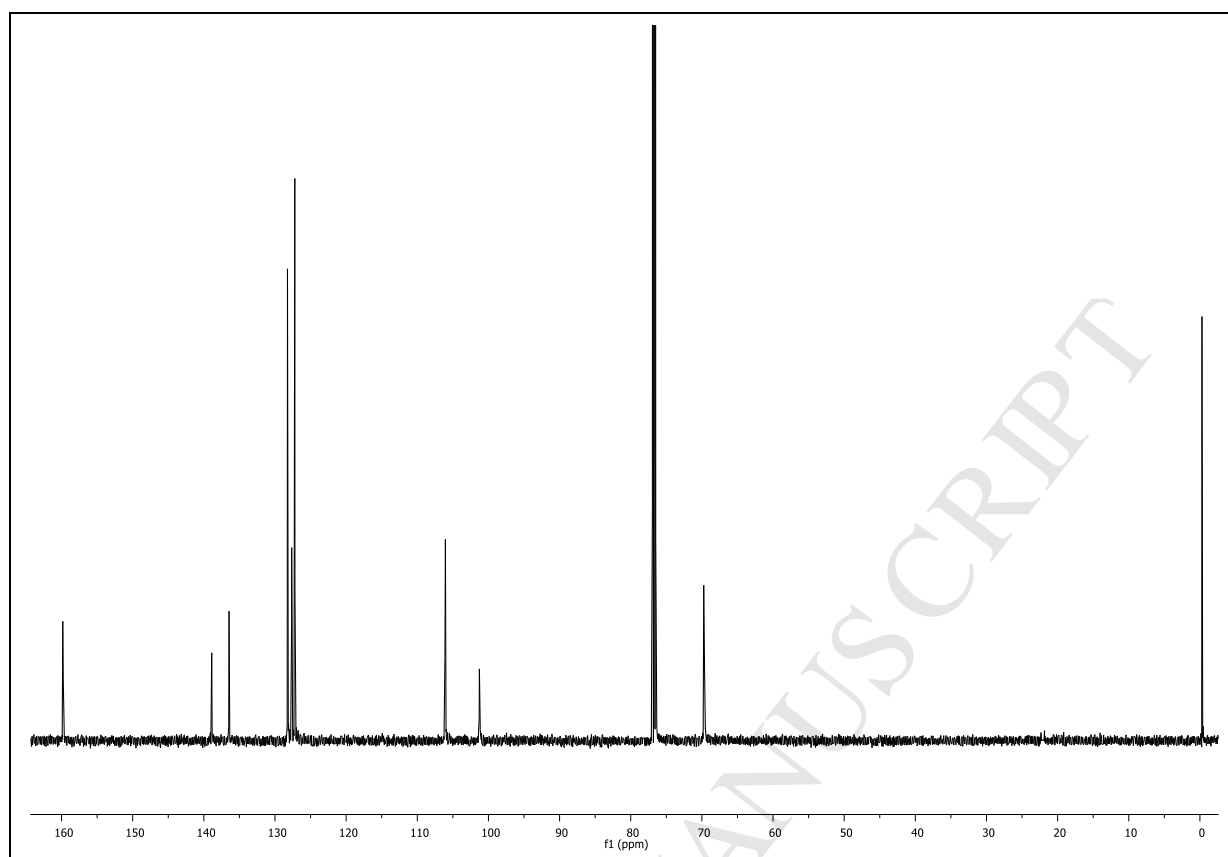
 $^{13}\text{C}$  NMR (CDCl<sub>3</sub>)

 $^1\text{H}$  NMR (CDCl<sub>3</sub>)

3e-G3

 $^{13}\text{C}$  NMR (CDCl<sub>3</sub>)



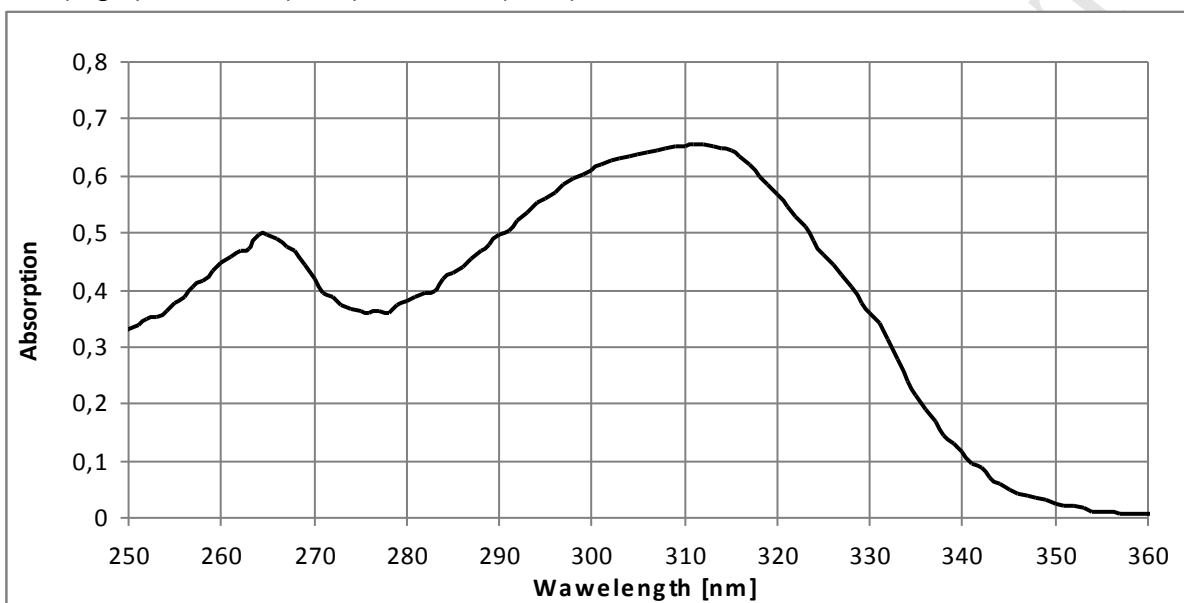


**UV-vis spectra of compounds:**

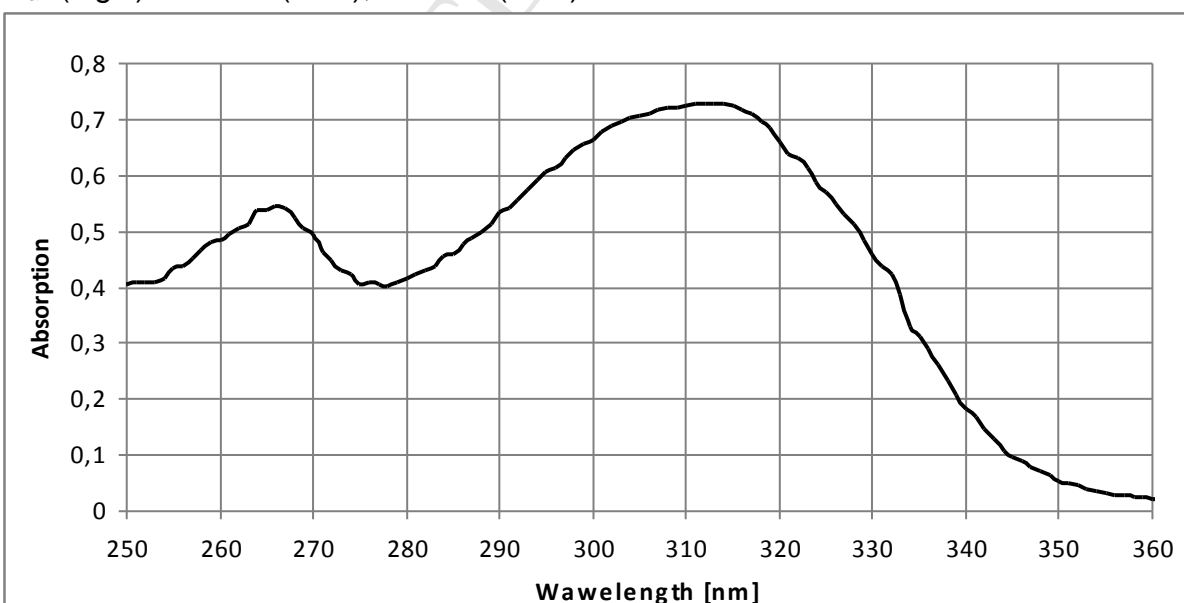
Spectra were measured in THF in standard 1 cm UV cell, with slit width of the spectrometer of 1 nm.

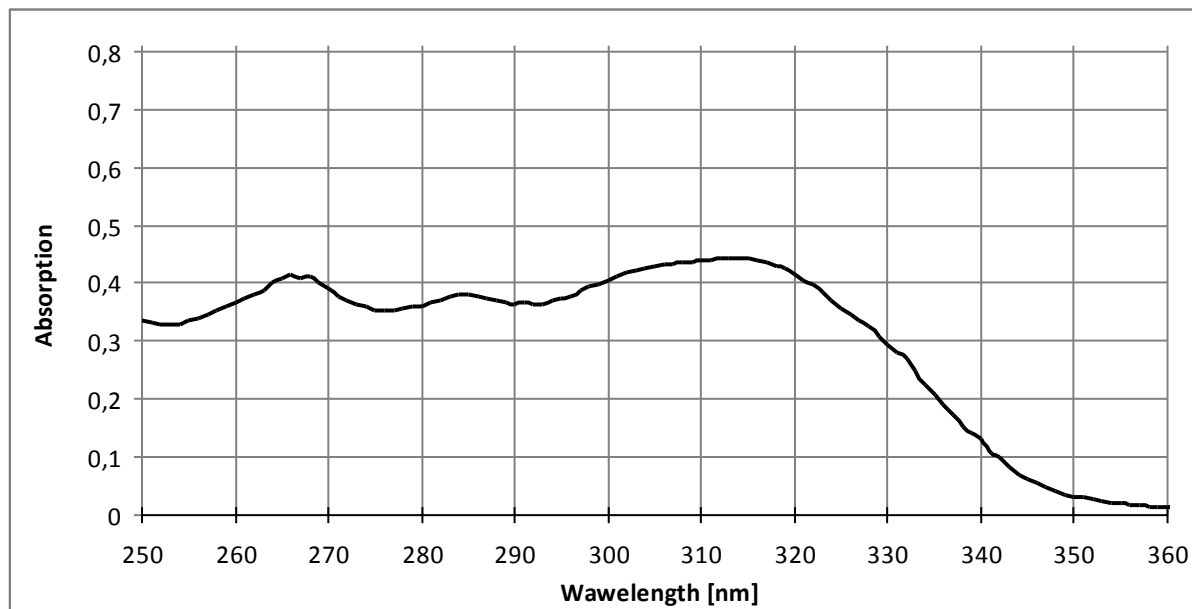
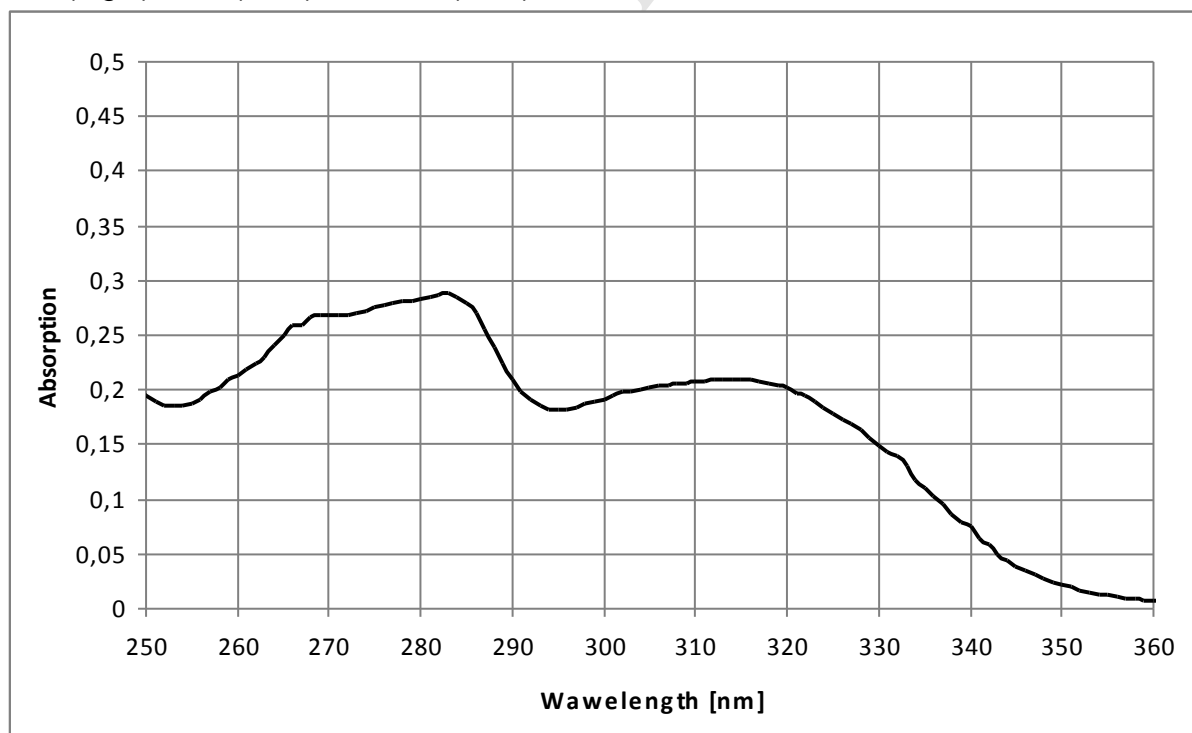
**3a**

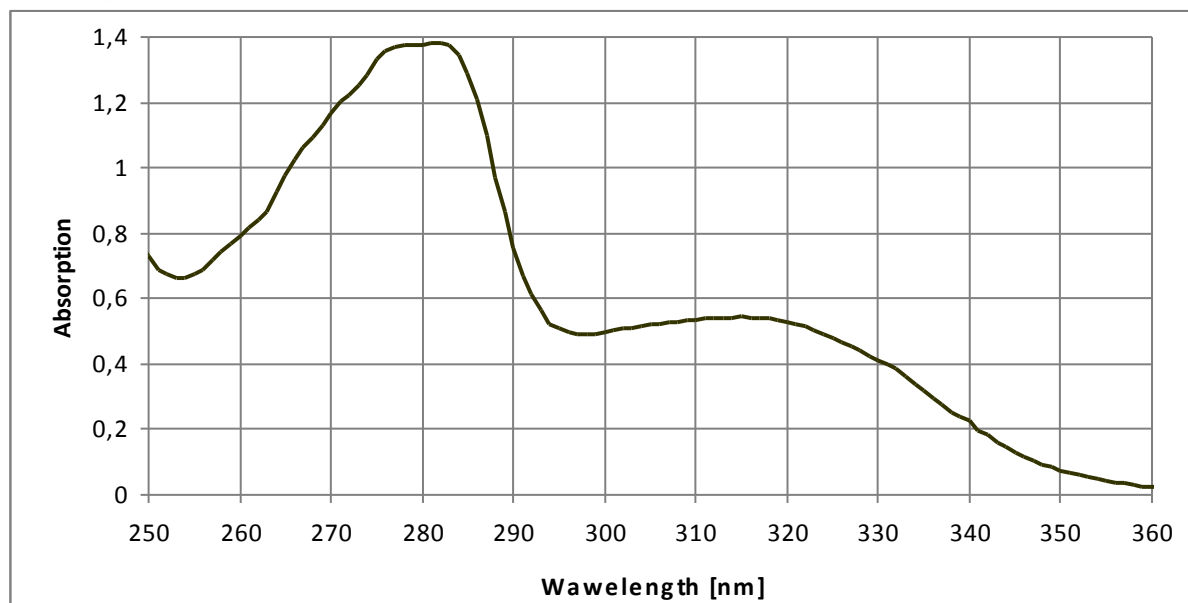
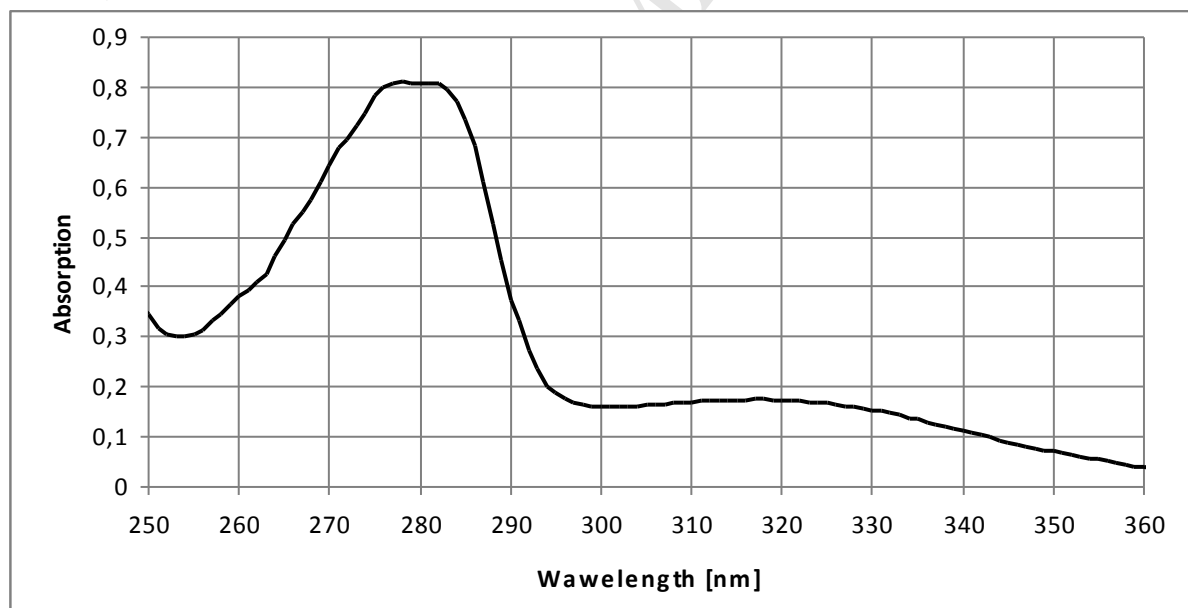
$\lambda_{\max}$  (log  $\epsilon$ ): 264 nm (4.14), 311 nm (4.26)

**3b-G0**

$\lambda_{\max}$  (log  $\epsilon$ ): 266 nm (4.26), 313 nm (4.39)

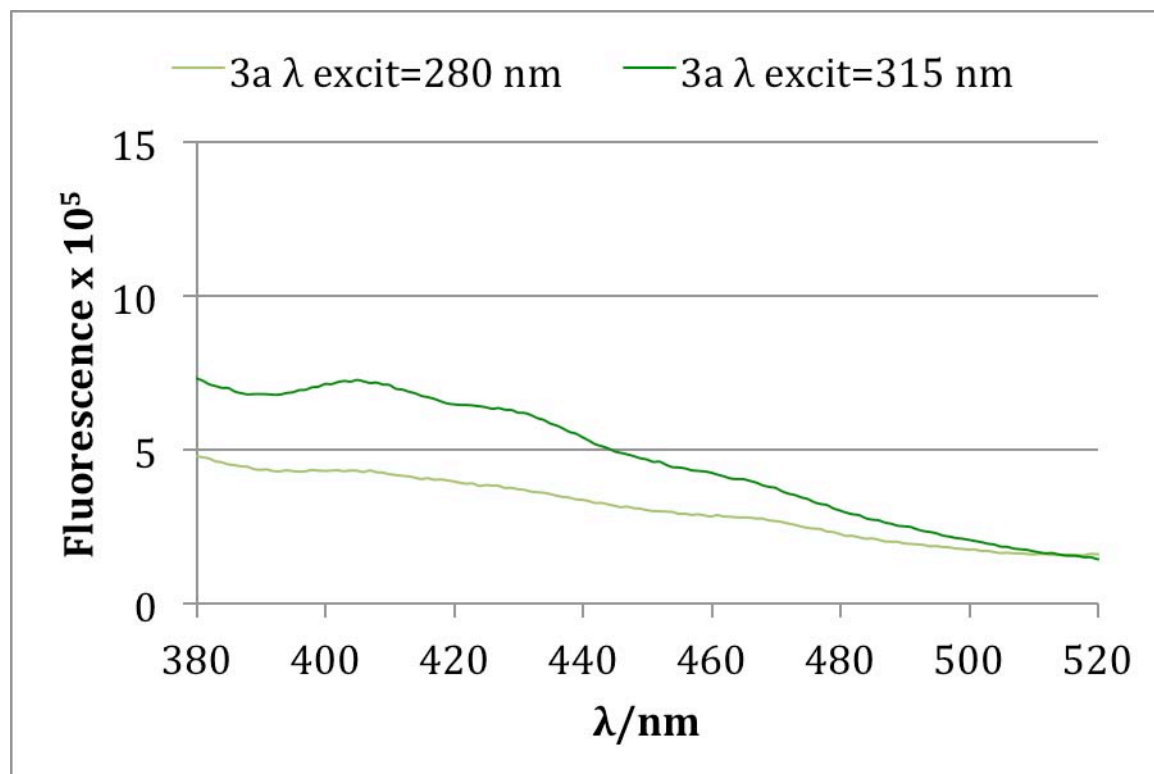


**3c-G1** $\lambda_{\max}$  (log  $\epsilon$ ): 266 nm (4.47), 284 nm (4.43), 315 nm (4.50)**3d-G2** $\lambda_{\max}$  (log  $\epsilon$ ): 283 (4.69), 315 nm (4.55)

**3e-G3** $\lambda_{\max}$  (log  $\epsilon$ ): 283 nm (4.69), 315 nm (4.55)**3f-G4** $\lambda_{\max}$  (log  $\epsilon$ ): 278 nm (5.27), 317 nm (4.60)

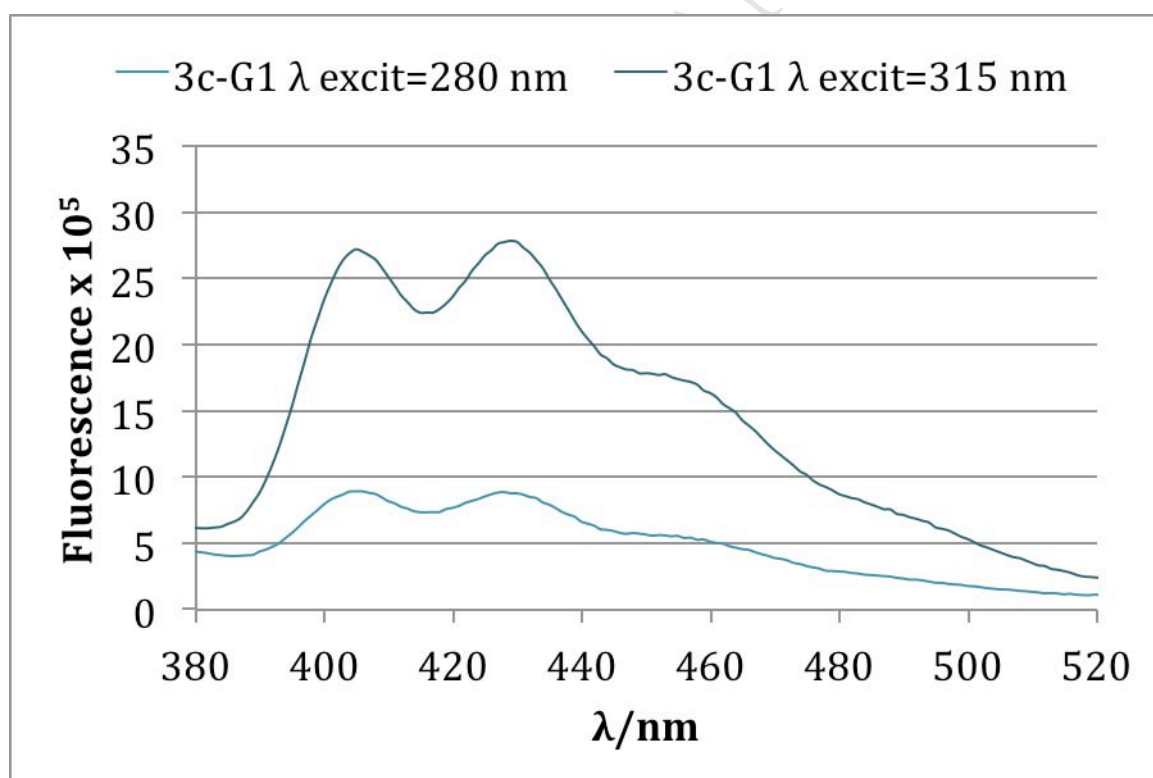
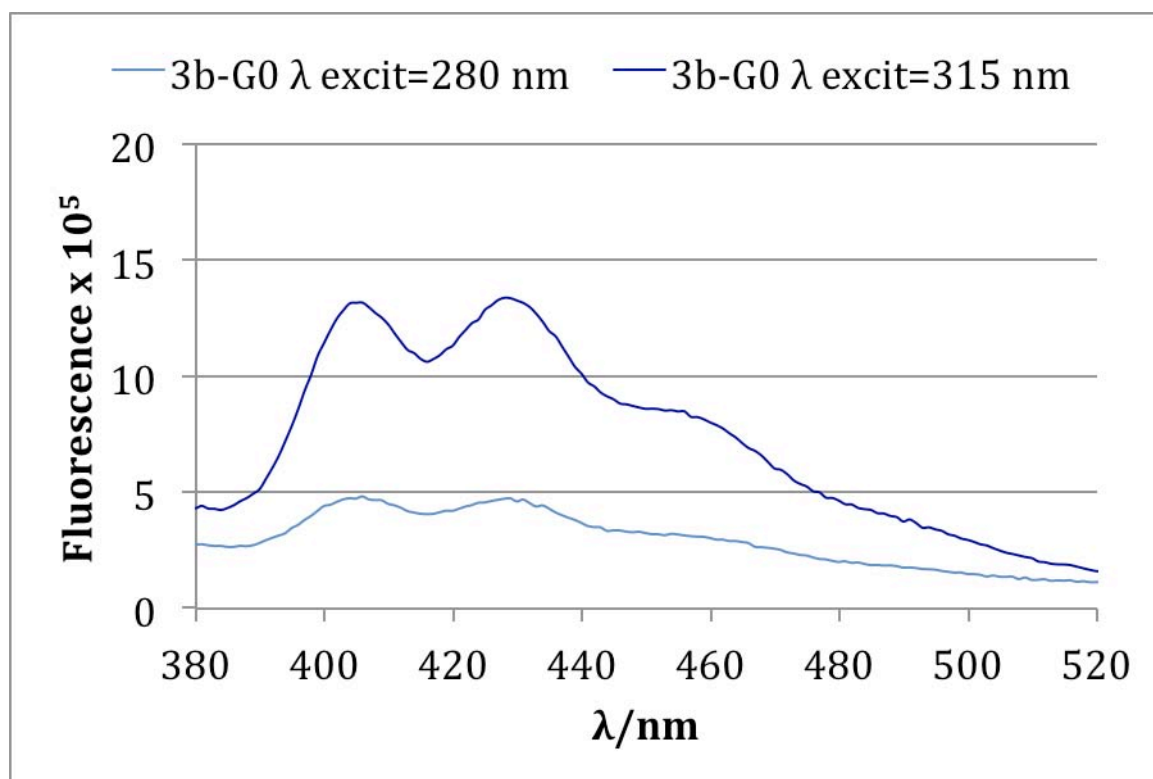
**Fluorescence spectra of compounds:**

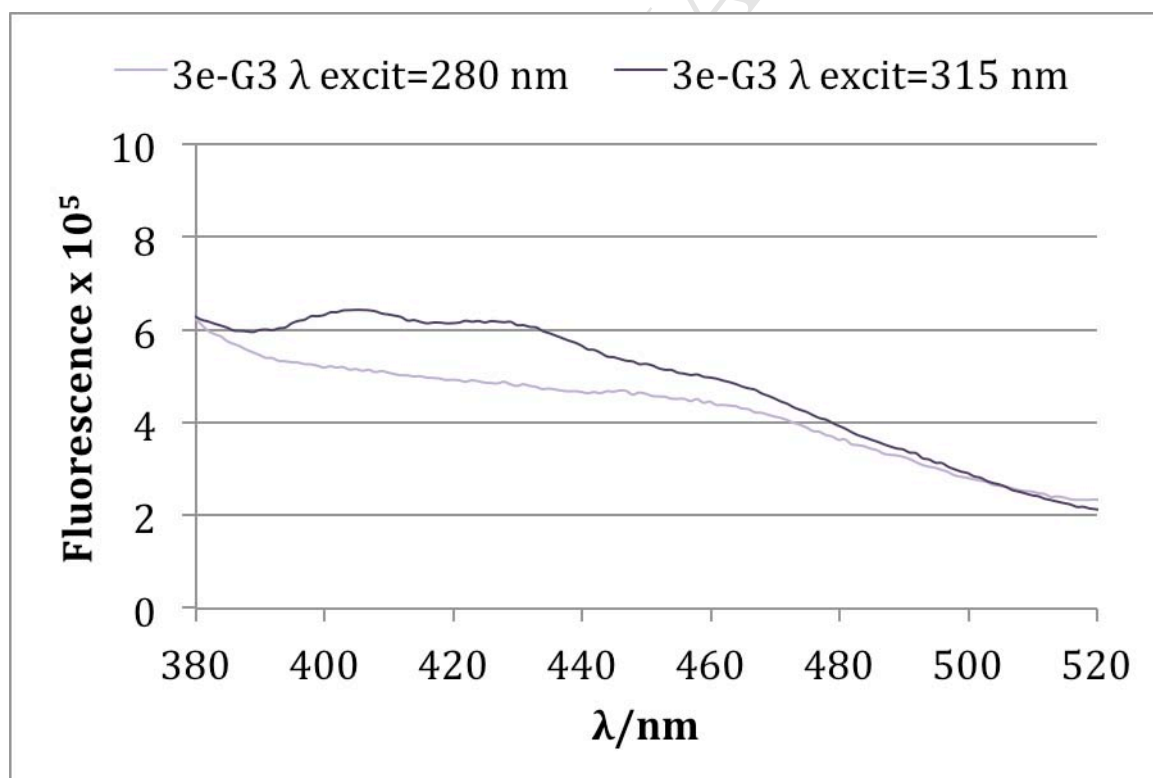
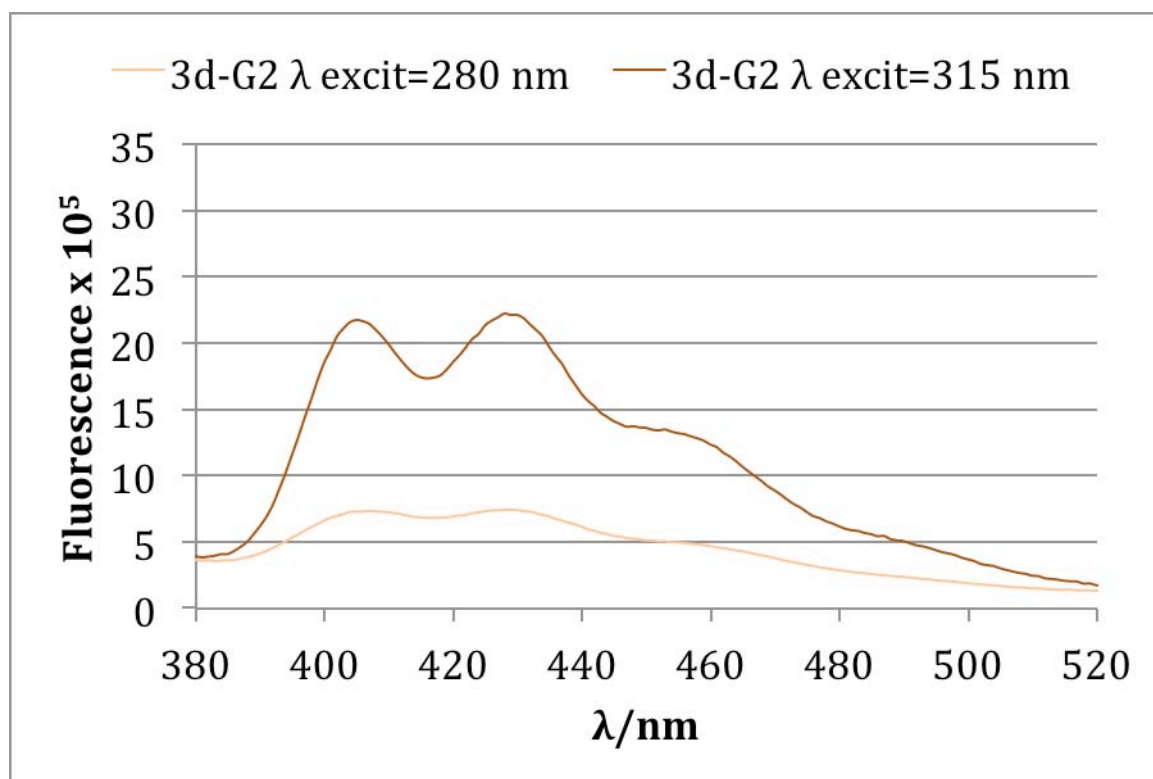
Spectra of THF solutions were determined by the method described by Williams (ref 35 in the main manuscript) (slit width: 10nm):

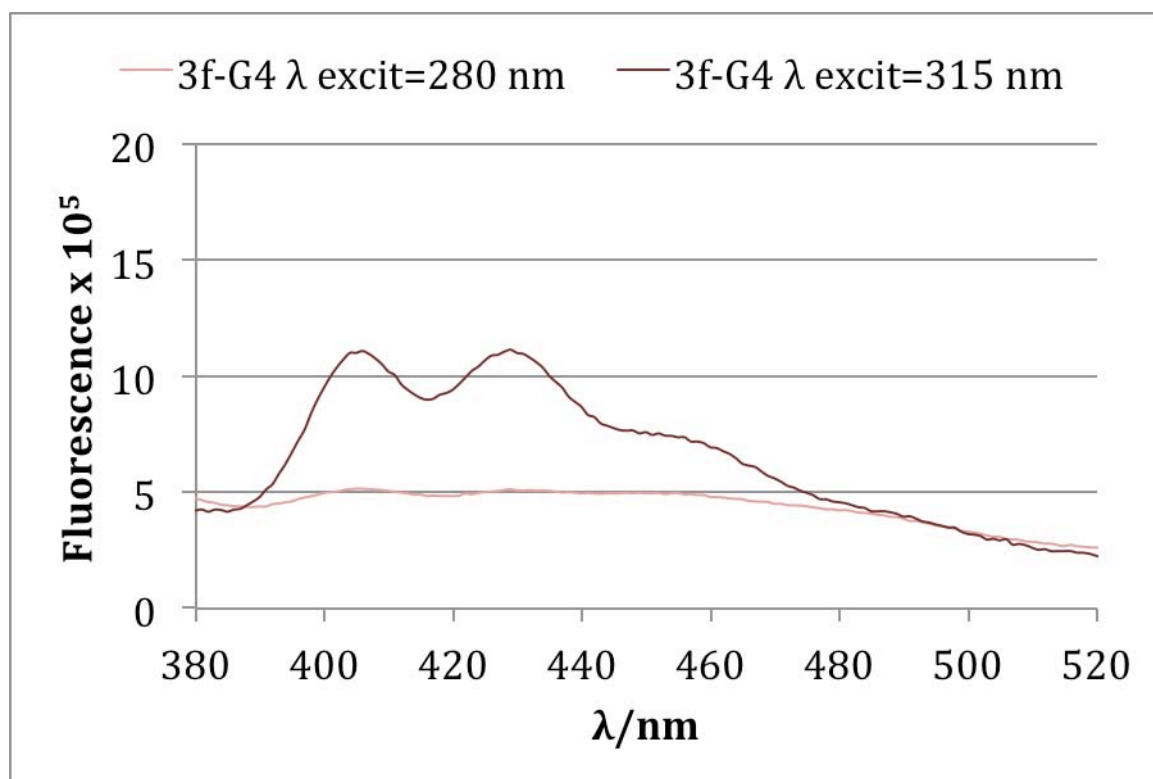


ACCEPTED









ACCEPTED MANUSCRIPT

**Relative RMSD for all the system**

D1:

Standard Deviation (SD) = 17.5251

RMSD = 4.1863

Average = 411.92

relative RMSD = RMSD/Average = 0.0101629

D2:

SD = 31.1404

RMSD = 5.58036

Average = 852.894

relative RMSD = RMSD/Average = 0.00654285

D3:

SD = 38.1543

RMSD = 6.17692

Average = 1673.54

relative RMSD = RMSD/Average = 0.00369093

D4:

SD = 56.255

RMSD = 7.50033

Average = 3321.03

relative RMSD = RMSD/Average = 0.00225843

D5:

SD = 76.3454

RMSD = 8.73759

Average = 6582.47

relative RMSD = RMSD/Average = 0.0013274

## Starting geometries of the MD simulations (Macromodel-Maestro format)

## 3b-G0

```

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64	41	5.801169	-5.009021	-2.780571	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
65	41	6.111823	-9.029126	1.045867	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
66	41	8.536366	-9.131132	0.452108	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
67	41	4.632028	-7.340757	-0.027231	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
68	41	9.474874	-7.532644	-1.222190	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
69	41	8.004433	-5.842671	-2.299169	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0

...

**3c-G1**

...

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3	2	1.020203	5.297933	1.527131	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
4	2	1.409475	2.627649	2.213640	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
5	2	1.189775	4.926505	2.863151	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
6	2	1.386160	3.594331	3.219088	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
7	2	1.011137	4.651249	-0.851359	1 " " X " "	2	0.32058	0.32058	" " " C " " "	6	0	0	1 C 0
8	2	1.048782	3.610859	-1.772405	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
9	16	1.289869	1.960338	-0.032946	1 " " X " "	70	-0.00030	-0.00030	" " " O " " "	8	0	0	1 O 0
10	2	1.164560	2.285350	-1.353860	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
11	2	1.576086	0.194272	-4.490428	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
12	2	0.940843	-0.989285	-4.114924	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
13	2	1.665182	1.264221	-3.597410	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
14	2	0.418280	-1.104196	-2.826161	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
15	2	1.125168	1.164778	-2.309126	1 " " X " "	2	0.00000	0.00000	" " " C " " "	6	0	0	1 C 0
16	2	0.511010	-0.036343	-1.934508	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
17	15	0.911487	5.791178	-1.245620	1 " " X " "	70	-0.32058	-0.32058	" " " O " " "	8	0	0	1 O 0
18	16	0.779050	6.608382	1.235105	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
19	16	1.539128	3.328012	4.551301	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
20	16	0.848533	-1.999773	-5.026692	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
21	3	-0.469542	7.120970	1.690759	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
22	2	-3.543518	5.005283	0.827138	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
23	2	-2.475304	5.563119	1.534230	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
24	2	-3.735149	5.364903	-0.509309	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
25	2	-1.610450	6.484863	0.927958	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
26	2	-2.875328	6.262299	-1.141409	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
27	2	-1.827433	6.829219	-0.412702	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
28	16	-4.349675	4.124019	1.494161	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
29	3	-5.489718	3.587193	0.834999	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
30	2	-7.925025	2.352020	3.499403	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
31	2	-7.264268	3.183527	2.594473	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
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33	2	-6.214473	2.690521	1.808156	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
34	2	-6.506863	0.513256	2.845026	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
35	2	-5.845111	1.346671	1.943357	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
36	16	-3.144332	6.548958	-2.451754	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
37	3	-2.091525	6.780354	-3.384660	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
38	2	-0.625072	4.460391	-6.020426	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
39	2	-1.059789	5.600982	-5.345297	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
40	2	-0.777690	3.203582	-5.439695	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
41	2	-1.658207	5.508084	-4.079680	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
42	2	-1.371570	3.093487	-4.184881	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
43	2	-1.807782	4.235360	-3.512089	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
44	3	1.205826	2.045960	5.068397	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
45	2	-0.263124	1.778032	4.839560	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
46	2	-0.702619	0.618674	4.189347	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
47	2	-1.216129	2.707441	5.272909	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
48	2	-2.063688	0.401485	3.957409	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
49	2	-2.578918	2.499659	5.062238	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
50	2	-2.995693	1.337531	4.407273	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
51	16	-3.421342	3.477344	5.512444	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
52	3	-4.789793	3.438334	5.136400	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
53	2	-5.935115	4.840826	6.904305	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
54	2	-5.430815	4.722456	5.603009	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
55	2	-6.533386	6.027488	7.329697	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
56	2	-5.535388	5.818971	4.736880	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
57	2	-6.634026	7.111228	6.458039	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0

58	2	-6.133475	7.005830	5.160934	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
59	16	-2.540753	-0.706531	3.315510	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
60	3	-1.908745	-1.142254	2.115692	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
61	2	-2.354258	-0.292323	0.947605	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
62	2	-1.936082	1.039145	0.817334	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
63	2	-3.188740	-0.829385	-0.043725	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
64	2	-2.339082	1.812010	-0.270882	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
65	2	-3.596108	-0.055365	-1.131059	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
66	2	-3.172219	1.266711	-1.245446	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
67	3	-0.462357	-2.480920	-5.299231	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
68	2	-1.754928	0.134067	-7.752933	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
69	2	-2.753400	0.750720	-6.996022	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
70	2	-1.031216	-0.922183	-7.194449	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
71	2	-3.021620	0.333430	-5.688632	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
72	2	-1.284585	-1.359424	-5.889691	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
73	2	-2.283839	-0.720313	-5.146982	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
74	16	-1.545062	0.628458	-9.011290	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
75	3	-0.412129	0.235618	-9.776901	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
76	2	3.244223	1.578958	-7.902967	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
77	2	2.176843	2.459702	-8.069206	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
78	2	3.131477	0.263452	-8.350054	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
79	2	0.999595	2.024325	-8.678379	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
80	2	1.953209	-0.170805	-8.958285	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
81	2	0.869017	0.702442	-9.123915	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
82	16	-3.958758	0.905908	-4.873851	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
83	3	-4.691207	2.037988	-5.322897	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
84	2	-7.258369	1.997571	-2.496708	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
85	2	-7.345654	3.351385	-2.176862	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
86	2	-6.398746	1.572527	-3.510081	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
87	2	-6.562810	4.276844	-2.865508	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
88	2	-5.605131	2.492067	-4.209166	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
89	2	-5.694415	3.849318	-3.870513	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
90	41	1.556861	1.565736	2.461365	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
91	41	1.161669	5.691907	3.655628	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
92	41	0.957307	3.857134	-2.841711	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
93	41	1.990902	0.289635	-5.507625	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
94	41	2.162981	2.191840	-3.923432	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
95	41	-0.073238	-2.034996	-2.501900	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
96	41	0.073614	-0.140533	-0.928039	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
97	41	-0.580887	6.976807	2.785485	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
98	41	-0.481287	8.219315	1.523731	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
99	41	-2.321743	5.272019	2.587143	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
100	41	-4.558629	4.936563	-1.097997	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
101	41	-1.154927	7.563429	-0.882296	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
102	41	-6.162155	4.406909	0.502877	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
103	41	-5.182968	3.004132	-0.058802	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
104	41	-8.745005	2.754202	4.118071	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
105	41	-7.568529	4.240449	2.509994	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
106	41	-8.068824	0.358559	4.341409	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
107	41	-6.201821	-0.542249	2.942509	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
108	41	-5.017740	0.942182	1.336776	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
109	41	-2.475696	7.492258	-4.146927	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
110	41	-1.220349	7.277250	-2.914846	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
111	41	-0.155332	4.554940	-7.012944	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
112	41	-0.921359	6.588154	-5.817364	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
113	41	-0.428439	2.298351	-5.965035	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
114	41	-1.487017	2.099186	-3.720762	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
115	41	-2.263678	4.120920	-2.517003	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
116	41	1.857151	1.265595	4.623873	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
117	41	1.413504	2.039421	6.159766	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
118	41	0.038407	-0.126705	3.862896	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
119	41	-0.890573	3.628909	5.784022	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
120	41	-4.062690	1.142595	4.224582	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
121	41	-4.877136	3.350187	4.035188	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
122	41	-5.294756	2.563208	5.598346	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
123	41	-5.858259	3.990566	7.602567	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
124	41	-6.925856	6.108667	8.357224	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0

125	41	-5.139992	5.748713	3.709473	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
126	41	-7.105798	8.049644	6.794265	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
127	41	-6.208383	7.861719	4.469387	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
128	41	-0.804023	-1.139312	2.206741	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
129	41	-2.193685	-2.201751	1.943008	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
130	41	-1.282532	1.494060	1.579221	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
131	41	-3.535784	-1.873406	0.030507	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
132	41	-1.998908	2.857698	-0.355022	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
133	41	-4.256885	-0.486298	-1.901845	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
134	41	-3.500009	1.878977	-2.101816	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
135	41	-0.390578	-3.317738	-6.026253	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
136	41	-0.929464	-2.903948	-4.386334	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
137	41	-3.310401	1.584229	-7.449722	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
138	41	-0.238153	-1.422820	-7.768717	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
139	41	-2.486881	-1.036679	-4.110618	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
140	41	-0.426309	-0.861452	-9.945292	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
141	41	-0.491261	0.702024	-10.782308	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
142	41	4.174767	1.921890	-7.420321	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
143	41	2.263897	3.501364	-7.717509	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
144	41	3.975147	-0.435368	-8.221139	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
145	41	0.161149	2.729371	-8.805062	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
146	41	1.882258	-1.214707	-9.306674	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
147	41	-3.993639	2.854546	-5.606679	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
148	41	-5.302657	1.772123	-6.212045	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H0
149	41	-7.874905	1.262508	-1.952221	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
150	41	-8.032865	3.687668	-1.382390	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
151	41	-6.348089	0.499747	-3.761578	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
152	41	-6.630170	5.349571	-2.616924	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0
153	41	-5.080599	4.594270	-4.405089	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H0

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**3d-G2**

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1	2	4.053107	2.264804	0.038453	1 " " X " "	2	0.00000	0.00000	" " C " "	"	6	0	0	1	C0
2	2	4.366407	1.491718	1.168665	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
3	2	3.357068	3.479368	0.212288	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
4	2	4.025053	1.937158	2.446050	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
5	2	3.002272	3.890036	1.501862	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
6	2	3.351798	3.141916	2.620663	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
7	2	4.440188	1.774353	-1.217713	1 " " X " "	2	0.32058	0.32058	" " C " "	"	6	0	0	1	C0
8	2	5.090055	0.543108	-1.276037	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
9	16	4.999435	0.282701	1.112175	1 " " X " "	70	-0.00030	-0.00030	" " O " "	"	8	0	0	1	O0
10	2	5.351556	-0.192723	-0.118568	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
11	2	7.263445	-3.249717	1.014253	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
12	2	7.184426	-4.083725	-0.099914	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
13	2	6.677249	-1.984529	0.990698	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
14	2	6.495532	-3.643368	-1.230392	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
15	2	5.991100	-1.524639	-0.140238	1 " " X " "	2	0.00000	0.00000	" " C " "	"	6	0	0	1	C0
16	2	5.903846	-2.376884	-1.249916	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
17	15	4.219410	2.378202	-2.243579	1 " " X " "	70	-0.32058	-0.32058	" " O " "	"	8	0	0	1	O0
18	16	3.050951	4.243936	-0.883085	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O0
19	16	3.016227	3.666304	3.833183	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O0
20	16	7.761389	-5.320271	-0.069594	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O0
21	3	2.087703	5.292459	-0.836844	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C0
22	2	2.020177	8.767308	0.734965	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
23	2	1.637046	7.584445	0.099037	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
24	2	3.341851	8.914063	1.162048	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
25	2	2.552633	6.548027	-0.129075	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C0
26	2	4.273167	7.897443	0.953303	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
27	2	3.871511	6.726618	0.304114	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
28	16	1.056443	9.724140	0.890689	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O0
29	3	1.392644	10.975348	1.475842	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C0
30	2	-0.970430	13.954498	1.131898	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
31	2	0.180146	13.162088	1.094888	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
32	2	-2.164031	13.398116	1.590965	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0
33	2	0.147265	11.828076	1.520540	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C0
34	2	-2.217438	12.079010	2.040414	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C0
35	2	-1.056791	11.301716	2.004901	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C0



36	16	5.542830	8.139215	1.401720	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
37	3	6.542069	7.130045	1.364342	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
38	2	7.136703	7.220850	-2.414339	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
39	2	6.883158	7.634402	-1.103691	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
40	2	7.382109	5.678254	-2.669708	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
41	2	6.866231	6.711865	-0.050126	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
42	2	7.372924	4.935376	-1.632547	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
43	2	7.119388	5.364639	-0.331425	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
44	3	3.708816	3.239630	4.999500	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
45	2	3.698672	4.362595	6.009631	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
46	2	4.101058	4.095590	7.321699	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
47	2	3.353611	5.678256	5.667938	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
48	2	4.178833	5.117376	8.266070	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
49	2	3.400901	6.708418	6.613366	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
50	2	3.819556	6.417931	7.913537	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
51	16	3.072861	8.008660	6.342106	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
52	3	2.669033	8.382678	5.030711	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
53	2	0.965677	10.231755	5.273287	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
54	2	2.295936	9.844867	5.071888	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
55	2	0.600836	11.578258	5.300305	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
56	2	3.269515	10.838283	4.907275	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
57	2	1.586919	12.552190	5.124153	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
58	2	2.923153	12.192571	4.938269	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
59	16	4.640494	4.832666	9.515989	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
60	3	6.030735	5.075814	9.701967	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
61	2	6.842690	4.191931	8.780916	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
62	2	7.187391	4.643166	7.499774	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
63	2	7.245904	2.910082	9.178232	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
64	2	7.910679	3.835110	6.620921	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
65	2	7.979382	2.091275	8.313310	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
66	2	8.301125	2.564804	7.041038	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
67	3	9.022332	-5.441981	-0.723253	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
68	2	11.921321	-5.199273	1.766878	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
69	2	12.063187	-3.816280	1.879523	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
70	2	10.945603	-5.736392	0.922950	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
71	2	11.225434	-2.968623	1.156521	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
72	2	10.109656	-4.897035	0.173727	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
73	2	10.281141	-3.513584	0.290695	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
74	16	12.727294	-5.997685	2.522329	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
75	3	12.095031	-6.605688	3.642166	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
76	2	10.239781	-3.509300	6.003841	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
77	2	9.459005	-4.284694	5.143001	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
78	2	11.609864	-3.755199	6.139472	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
79	2	10.068829	-5.290919	4.388000	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
80	2	12.196579	-4.772823	5.384893	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
81	2	11.441060	-5.542211	4.494468	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
82	16	11.260322	-1.611730	1.273853	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
83	3	11.313882	1.077941	2.596028	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
84	2	8.025749	0.637241	3.510989	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
85	2	8.195634	1.875128	2.892537	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
86	2	9.040454	-0.318699	3.411599	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
87	2	9.365990	2.180998	2.199054	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
88	2	10.217505	-0.043296	2.701366	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
89	2	10.369344	1.212672	2.099118	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
90	16	7.143447	8.052457	-3.500157	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
91	16	7.590112	3.598001	-1.793131	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
92	16	-3.426503	11.637965	2.499961	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
93	16	-1.018496	15.265974	0.748690	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
94	16	-0.721844	11.849935	5.512648	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
95	16	3.811134	13.224132	4.805987	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
96	16	8.406816	0.828137	8.615995	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
97	16	8.274117	4.199183	5.354084	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
98	16	9.450190	3.440665	1.675885	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
99	16	6.851690	0.460382	4.186121	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
100	16	8.116935	-4.020881	5.095711	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
101	16	12.442783	-3.091313	6.996490	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
102	3	7.886901	3.072957	-3.077793	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0

103	2	8.170854	1.597656	-2.929661	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
104	3	-1.168551	13.197218	5.585525	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
105	2	-2.980922	12.661424	7.259438	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
106	2	-2.618454	13.173374	6.006176	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
107	2	-4.316898	12.639139	7.661313	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
108	2	-3.624610	13.665771	5.165709	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
109	2	-5.309277	13.128026	6.812924	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
110	2	-4.961336	13.640007	5.563887	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
111	3	5.208370	12.992976	4.691536	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
112	2	5.573136	12.435837	3.335436	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
113	2	6.682117	11.589485	3.199058	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
114	2	4.834945	12.763780	2.190238	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
115	2	7.037041	11.073201	1.953404	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
116	2	5.192526	12.252876	0.943048	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
117	2	6.292212	11.405197	0.823691	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
118	3	8.056054	0.228520	9.854852	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
119	2	8.632185	-1.167082	9.853287	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
120	2	9.791785	-1.468114	10.580370	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
121	2	8.011412	-2.189477	9.122375	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
122	2	10.317523	-2.760752	10.578812	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
123	2	8.537575	-3.481802	9.119799	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
124	2	9.691572	-3.768806	9.847102	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
125	3	7.558280	5.207648	4.652606	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
126	2	6.868899	7.565585	5.219881	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
127	2	7.878118	6.595531	5.154912	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
128	2	7.140779	8.844875	5.702433	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
129	2	9.170650	6.942138	5.569566	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
130	2	8.430849	9.178052	6.111876	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
131	2	9.446322	8.225416	6.042230	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
132	3	10.691368	3.922963	1.179567	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
133	2	10.442126	5.966618	-0.305453	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
134	2	10.545223	5.411481	0.976009	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
135	2	10.304961	7.344954	-0.473964	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
136	2	10.510120	6.268096	2.084322	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
137	2	10.268476	8.186615	0.637013	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
138	2	10.371220	7.646247	1.918063	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
139	3	6.631797	-0.692712	4.985804	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
140	2	4.111220	-0.837044	4.890780	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
141	2	5.268737	-0.515233	5.610135	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
142	2	2.848429	-0.658073	5.456314	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
143	2	5.133130	-0.011574	6.909361	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
144	2	2.727257	-0.164404	6.754407	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
145	2	3.872241	0.158222	7.481187	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
146	3	7.253889	-5.029548	4.583199	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
147	2	4.904038	-4.576712	3.756776	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
148	2	5.819061	-4.626413	4.817385	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
149	2	3.566401	-4.254149	3.986247	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
150	2	5.366547	-4.335777	6.110930	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
151	2	3.126868	-3.976246	5.279618	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
152	2	4.029975	-4.010113	6.340975	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
153	3	12.108715	-1.826262	7.552908	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
154	2	13.646276	-0.632711	5.940311	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
155	2	12.388540	-0.732736	6.550258	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
156	2	13.925367	0.401450	5.046354	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
157	2	11.415272	0.225829	6.243402	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
158	2	12.950053	1.353574	4.754298	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
159	2	11.694574	1.263841	5.353331	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
160	3	0.172815	16.030645	0.619927	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
161	2	0.179126	16.372799	3.132200	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
162	2	0.890331	16.143711	1.946010	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0
163	2	0.844099	16.481607	4.353700	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
164	2	2.286445	16.036196	2.011793	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
165	2	2.232388	16.368069	4.405421	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
166	2	2.952730	16.147388	3.232646	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
167	3	-3.520015	10.374284	3.142402	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1 C 0
168	2	-5.986908	10.082649	2.677500	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1 C 0
169	2	-4.945652	10.201091	3.607195	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1 C 0

170	2	-7.305923	9.920245	3.102560	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
171	2	-5.254241	10.152332	4.972744	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
172	2	-7.600464	9.873729	4.464603	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
173	2	-6.572705	9.990632	5.399305	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
174	3	6.725989	9.407447	-3.402005	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
175	2	4.334432	8.509818	-3.321325	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
176	2	5.249623	9.550032	-3.105505	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
177	2	2.979075	8.680564	-3.039690	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
178	2	4.764767	10.770977	-2.613982	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
179	2	2.514122	9.896111	-2.542382	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
180	2	3.408962	10.942913	-2.332512	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
181	2	8.812330	1.100326	-1.787763	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
182	2	9.084492	-0.259741	-1.660059	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
183	2	8.723780	-1.143555	-2.675644	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
184	2	7.809630	0.699284	-3.942913	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
185	2	8.083942	-0.662826	-3.816957	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
186	41	4.292695	1.317502	3.314727	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
187	41	2.461108	4.833329	1.668905	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
188	41	5.395699	0.162878	-2.262732	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
189	41	7.807564	-3.582521	1.912431	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
190	41	6.764045	-1.339464	1.879082	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
191	41	6.411319	-4.300722	-2.111343	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
192	41	5.354372	-2.062504	-2.151444	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
193	41	1.835502	5.561899	-1.885309	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
194	41	1.146663	4.911998	-0.384464	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
195	41	0.592858	7.476389	-0.238256	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
196	41	3.678873	9.832145	1.666553	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
197	41	4.594936	5.921181	0.120015	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
198	41	1.774868	10.830235	2.506226	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
199	41	2.181921	11.472972	0.873367	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
200	41	1.129866	13.579144	0.728392	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
201	41	-3.076054	14.016325	1.616067	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
202	41	-1.071410	10.258079	2.354509	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
203	41	7.460399	7.528324	1.844505	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
204	41	6.213629	6.266399	1.980663	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
205	41	6.672653	8.691253	-0.884244	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
206	41	7.569964	5.561446	-3.708736	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
207	41	7.106518	4.619324	0.481225	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
208	41	3.219990	2.331802	5.409660	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
209	41	4.768354	2.998537	4.764908	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
210	41	4.397569	3.073175	7.607615	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
211	41	3.049401	5.896000	4.633110	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
212	41	3.875660	7.224961	8.661551	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
213	41	3.496002	8.215455	4.307770	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
214	41	1.795708	7.778647	4.704055	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
215	41	0.185550	9.465130	5.413833	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
216	41	4.314512	10.532666	4.749489	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
217	41	1.331772	13.622370	5.134581	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
218	41	6.258451	6.149826	9.531253	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
219	41	6.290513	4.867219	10.761424	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
220	41	6.867020	5.649714	7.192728	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
221	41	6.968721	2.557456	10.183307	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
222	41	8.861884	1.920535	6.346887	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
222	41	8.861884	1.920535	6.346887	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
223	41	9.206479	-6.516197	-0.937132	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
224	41	9.011036	-4.923646	-1.705569	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
225	41	12.826351	-3.403661	2.558518	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
226	41	10.833838	-6.830209	0.851926	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
227	41	9.632019	-2.832984	-0.280017	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
228	41	11.357482	-7.362267	3.300252	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
229	41	12.858795	-7.156230	4.231238	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
230	41	9.746210	-2.720822	6.590764	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
231	41	9.479737	-5.895531	3.682015	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
232	41	13.278632	-4.959242	5.486601	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
233	41	11.170306	-1.865380	3.365622	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
234	41	12.311486	-0.623420	2.767701	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
235	41	7.396268	2.629764	2.967913	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0

236	41	8.926026	-1.304558	3.888595	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
237	41	11.297363	1.422417	1.545382	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
238	41	7.026401	3.237833	-3.761007	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
239	41	8.784170	3.573312	-3.502175	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
240	41	-0.583305	13.763042	6.341988	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
241	41	-1.042406	13.694446	4.600463	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
242	41	-2.203906	12.269022	7.936990	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
243	41	-4.588704	12.231277	8.649207	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
244	41	-3.366118	14.074891	4.175591	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
245	41	-6.366702	13.105539	7.125020	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
246	41	-5.744566	14.020544	4.886928	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
247	41	5.731024	13.964846	4.822903	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
248	41	5.556124	12.340065	5.519701	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
249	41	7.288092	11.324797	4.080960	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
250	41	3.960870	13.431529	2.268132	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
251	41	7.907237	10.401522	1.862344	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
252	41	4.602246	12.517940	0.050937	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
253	41	6.571893	10.996361	-0.160408	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
254	41	8.466850	0.821126	10.699761	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
255	41	6.951436	0.182249	9.966391	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
256	41	10.300038	-0.679922	11.160954	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
257	41	7.099256	-1.976239	8.539724	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
258	41	11.231003	-2.985582	11.154819	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
259	41	8.043717	-4.278467	8.538695	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
260	41	10.108918	-4.789884	9.841051	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
261	41	7.843033	5.150651	3.580468	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
262	41	6.469527	4.993424	4.697103	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
263	41	5.843425	7.316826	4.899895	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
264	41	6.331282	9.590291	5.764660	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
265	41	9.980441	6.194290	5.532378	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
266	41	8.646941	10.189506	6.494464	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
267	41	10.467725	8.483189	6.369168	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
268	41	11.506050	3.731673	1.911138	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
269	41	10.949010	3.410194	0.228724	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
270	41	10.457980	5.313671	-1.194090	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
271	41	10.215242	7.767183	-1.488951	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
272	41	10.588649	5.849740	3.101194	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
273	41	10.154912	9.274956	0.501743	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
274	41	10.338729	8.307090	2.800776	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
275	41	6.653224	-1.611040	4.362324	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
276	41	7.417487	-0.780360	5.766338	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
277	41	4.195304	-1.236253	3.865617	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
278	41	1.945727	-0.912337	4.876036	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
279	41	6.029830	0.259472	7.487932	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
280	41	1.729225	-0.026277	7.203099	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
281	41	3.780731	0.553898	8.506664	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
282	41	7.437892	-5.178968	3.499271	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
283	41	7.443689	-5.995338	5.100669	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
284	41	5.232615	-4.803316	2.728250	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
285	41	2.855291	-4.222031	3.143680	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
286	41	6.068428	-4.370135	6.960244	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
287	41	2.069623	-3.722057	5.462775	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
288	41	3.686065	-3.779855	7.363342	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
289	41	11.065318	-1.809611	7.921611	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
290	41	12.749219	-1.658988	8.445499	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
291	41	14.429190	-1.374390	6.172286	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
292	41	14.920130	0.468946	4.574804	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
293	41	10.420588	0.168285	6.714919	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
294	41	13.168729	2.174311	4.050922	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
295	41	10.921676	2.015599	5.120057	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
296	41	0.818900	15.599241	-0.172807	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
297	41	-0.101912	17.050146	0.273809	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1 H 0
298	41	-0.919770	16.466816	3.105924	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
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301	41	2.759225	16.453579	5.370561	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1 H 0
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304 41 -2.818677 10.328366 4.002791 1 " " X " " 21 0.00000 0.00000 " " " H " " " 1 0 0 1 H 0
305 41 -5.764901 10.121809 1.597759 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
306 41 -8.116508 9.830030 2.360097 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
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308 41 -8.642810 9.746581 4.801394 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
309 41 -6.800982 9.958224 6.477794 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
310 41 7.345681 9.938445 -2.648722 1 " " X " " 21 0.00000 0.00000 " " " H " " " 1 0 0 1 H 0
311 41 6.935694 9.901422 -4.375338 1 " " X " " 21 0.00000 0.00000 " " " H " " " 1 0 0 1 H 0
312 41 4.677433 7.538249 -3.714176 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
313 41 2.274464 7.849674 -3.208232 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
314 41 5.458990 11.611466 -2.449194 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
315 41 1.442964 10.027643 -2.315055 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
316 41 3.041023 11.907146 -1.944963 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
317 41 9.107198 1.783306 -0.973611 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
318 41 9.585840 -0.628145 -0.750546 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
319 41 8.941000 -2.219557 -2.575814 1 " " X " " 21 0.11346 0.11346 " " " H " " " 1 0 0 1 H 0
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### 3e-G3

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2 2 0.433798 -1.558429 -4.165342 1 " " X " " 2 0.00015 0.00015 " " " C " " " 6 0 0 1 C 0
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4 2 0.382094 -2.021444 -5.482871 1 " " X " " 2 -0.11346 -0.11346 " " " C " " " 6 0 0 1 C 0
5 2 -0.673528 0.021840 -6.166061 1 " " X " " 2 -0.11346 -0.11346 " " " C " " " 6 0 0 1 C 0
6 2 -0.163639 -1.232757 -6.494338 1 " " X " " 2 0.00015 0.00015 " " " C " " " 6 0 0 1 C 0
7 2 0.010057 0.129661 -2.501264 1 " " X " " 2 0.32058 0.32058 " " " C " " " 6 0 0 1 C 0
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22 2 3.846583 -7.874337 2.531053 1 " " X " " 2 -0.12501 -0.12501 " " " C " " " 6 0 0 1 C 0
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35 2 11.547411 -9.183036 0.787901 1 " " X " " 2 0.00015 0.00015 " " " C " " " 6 0 0 1 C 0
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37 2 11.237360 -9.844954 -0.403065 1 " " X " " 2 -0.11346 -0.11346 " " " C " " " 6 0 0 1 C 0
38 2 2.495807 -8.170708 6.876195 1 " " X " " 2 -0.12501 -0.12501 " " " C " " " 6 0 0 1 C 0
39 2 1.322025 -8.041926 7.632553 1 " " X " " 2 -0.11346 -0.11346 " " " C " " " 6 0 0 1 C 0
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42 2 2.790397 -5.749911 7.001211 1 " " X " " 2 0.00015 0.00015 " " " C " " " 6 0 0 1 C 0
43 2 1.633193 -5.654810 7.774914 1 " " X " " 2 -0.11346 -0.11346 " " " C " " " 6 0 0 1 C 0
44 16 12.721207 -8.512113 0.990835 1 " " X " " 70 -0.17255 -0.17255 " " " O " " " 8 0 0 1 O 0
45 16 9.745663 -11.016546 -1.797892 1 " " X " " 70 -0.17255 -0.17255 " " " O " " " 8 0 0 1 O 0

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46	16	-0.224954	-6.639145	8.860733	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
47	16	3.420188	-4.585223	6.649687	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
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49	3	-1.442887	-7.241310	8.434719	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
50	3	4.277455	-4.609719	5.510669	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
51	3	8.454203	-10.863643	-2.380874	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
52	2	12.387885	-6.863509	-0.726713	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
53	2	11.904479	-7.022899	-2.031934	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
54	2	11.950400	-5.763016	0.022405	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
55	2	10.994502	-6.119543	-2.582150	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
56	2	11.044719	-4.843723	-0.515503	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
57	2	10.576081	-5.029090	-1.816612	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
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59	2	6.224116	-11.487813	-1.339323	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
60	2	7.848767	-13.222632	-1.749244	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
61	2	5.354651	-12.428370	-0.778855	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
62	2	6.992863	-14.169739	-1.184151	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
63	2	5.741061	-13.767248	-0.720074	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
64	2	-1.978591	-6.512891	7.224380	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
65	2	-2.056875	-5.114687	7.231384	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
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68	2	-2.913820	-6.524956	4.974091	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	0	0
69	2	-2.971481	-5.128985	5.002543	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
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71	2	4.992033	-3.174994	3.601363	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
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90	3	-3.741036	-6.618866	2.721087	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
91	3	3.642002	1.564664	4.863340	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
92	2	10.062187	-2.385360	2.022365	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
93	2	9.120980	-2.526459	3.051053	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
94	2	10.259818	-1.116249	1.462143	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
95	2	8.401193	-1.424392	3.513137	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
96	2	9.535467	-0.014693	1.919222	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
97	2	8.606705	-0.167117	2.947625	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
98	2	9.267373	-6.076044	-5.827992	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
99	2	10.278172	-6.495185	-6.703974	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
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102	2	7.620675	-6.664613	-7.515604	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
103	2	8.634956	-7.082036	-8.375672	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
104	2	2.731845	-10.876436	1.207142	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
105	2	2.651716	-11.555858	2.429509	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
106	2	1.595594	-10.205438	0.738281	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
107	2	1.465838	-11.562126	3.164794	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
108	2	0.410159	-10.206998	1.472664	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
109	2	0.343597	-10.885276	2.688671	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
110	2	9.120307	-15.001145	0.530638	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
111	2	8.423004	-15.128428	1.739698	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
112	2	10.211341	-14.122215	0.475815	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0



113	2	8.800826	-14.391259	2.862606	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
114	2	10.588699	-13.383193	1.597342	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
115	2	9.883624	-13.516026	2.792207	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
116	2	-1.791817	-0.846653	6.438535	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
117	2	-2.386406	-0.446364	5.233747	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
118	2	-1.005197	0.080190	7.137446	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
119	2	-2.192279	0.841951	4.739744	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
120	2	-0.812486	1.370392	6.643820	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
121	2	-1.403526	1.750479	5.440956	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
122	2	2.785174	1.725202	3.626952	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
123	2	1.481117	1.216471	3.583198	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
124	2	3.271273	2.411275	2.504123	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
125	2	0.684609	1.382429	2.449622	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
126	2	2.476618	2.576294	1.368465	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
127	2	1.180789	2.063833	1.340230	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
128	2	5.794448	-1.346963	-0.619846	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
129	2	7.045781	-1.873388	-0.963153	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
130	2	4.810757	-1.250357	-1.613611	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
131	2	7.304188	-2.296577	-2.267301	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
132	2	5.067254	-1.675955	-2.916739	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
133	2	6.315689	-2.201466	-3.246010	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
134	2	-4.068475	-7.629210	1.647803	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
135	2	-5.029718	-7.322895	0.674388	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
136	2	-3.410481	-8.864086	1.575657	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
137	2	-5.324280	-8.226785	-0.346368	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
138	2	-3.706059	-9.770669	0.556908	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
139	2	-4.662266	-9.452148	-0.406517	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
140	3	0.143939	-2.889225	-8.255299	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
141	2	-0.841946	-3.945593	-7.810421	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
142	2	-0.389782	-5.225511	-7.474364	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
143	2	-2.218052	-3.689019	-7.760866	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
144	2	-1.274595	-6.226106	-7.069740	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
145	2	-3.125205	-4.680832	-7.369049	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
146	2	-2.642414	-5.942717	-7.009057	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
147	16	-4.483234	-4.498916	-7.331356	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
148	16	-0.709207	-7.434691	-6.773184	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
149	3	-5.046893	-3.352225	-7.957975	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
150	3	-1.476913	-8.517020	-6.263002	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
151	2	-0.558594	-9.717449	-6.272240	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
152	2	-0.265391	-10.341655	-7.490455	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
153	2	0.035199	-10.213387	-5.103595	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
154	2	0.608910	-11.426739	-7.556680	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
155	2	0.903872	-11.309147	-5.152200	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
156	2	1.180700	-11.912769	-6.379950	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
157	2	-6.558263	-3.385691	-7.902247	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
158	2	-7.296377	-2.689848	-8.870237	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
159	2	-7.252542	-4.053424	-6.883959	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
160	2	-8.691200	-2.645524	-8.815830	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
161	2	-8.650442	-4.028395	-6.822914	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
162	2	-9.358090	-3.321240	-7.795646	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
163	16	0.889127	-11.911324	-8.804186	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
164	16	1.513755	-11.861770	-4.061073	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
165	16	-9.443911	-1.952391	-9.721334	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
166	16	-9.403354	-4.640713	-5.858095	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
167	3	2.129521	-12.553521	-9.077931	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
168	3	-9.112103	-0.584765	-9.935973	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
169	3	-8.845756	-5.626690	-4.999996	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
170	3	1.890238	-11.062966	-2.947682	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
171	2	3.328586	-11.628253	-9.010813	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
172	2	4.565861	-12.098083	-9.472227	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
173	2	3.269147	-10.317013	-8.519869	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
174	2	5.706893	-11.293324	-9.451017	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
175	2	4.401434	-9.501170	-8.469184	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
176	2	5.618242	-9.995587	-8.939635	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
177	2	3.035605	-10.139211	-3.299848	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
178	2	3.113272	-8.852548	-2.752105	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
179	2	4.067542	-10.563684	-4.146911	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0

180	2	4.165843	-7.987227	-3.056622	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
181	2	5.134457	-9.716102	-4.454921	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
182	2	5.164246	-8.426112	-3.926422	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
183	2	-9.231446	0.162473	-8.627954	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
184	2	-10.472229	0.620155	-8.164255	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
185	2	-8.099305	0.371770	-7.833251	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
186	2	-10.582703	1.273148	-6.931003	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
187	2	-8.199936	0.991679	-6.591022	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
188	2	-9.439878	1.451886	-6.148967	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
189	2	-7.950202	-5.011960	-3.950346	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
190	2	-6.683842	-5.556715	-3.715881	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
191	2	-8.350728	-3.898591	-3.200461	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
192	2	-5.819349	-4.998116	-2.777611	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
193	2	-7.504167	-3.339248	-2.237111	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
194	2	-6.238068	-3.892883	-2.034190	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
195	16	6.852712	-11.849710	-9.946805	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
196	16	4.387344	-8.221682	-7.983686	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
197	16	4.121631	-6.748183	-2.477985	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
198	16	6.199247	-10.064111	-5.234058	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
199	16	-11.754713	1.745592	-6.409859	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
200	16	-7.060052	1.086040	-5.851075	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
201	16	-4.591313	-5.583210	-2.688287	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
202	16	-7.820194	-2.252746	-1.469830	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
203	3	3.184174	-7.685377	-7.445040	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
204	3	8.029434	-11.063494	-10.074482	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
205	3	5.159299	-5.779033	-2.604742	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
206	3	6.407557	-11.416022	-5.620060	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
207	3	-12.986212	1.507164	-7.075741	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
208	3	-3.567823	-5.004128	-1.894836	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
209	3	-7.162472	0.744454	-4.472095	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
210	3	-9.099705	-1.644064	-1.570525	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
211	2	3.432088	-6.246974	-7.055843	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
212	2	3.932071	-5.332067	-7.991681	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
213	2	3.139722	-5.792415	-5.763726	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
214	2	4.144550	-3.998475	-7.641435	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
215	2	3.346693	-4.458212	-5.412915	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
216	2	3.851138	-3.559418	-6.351464	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
217	2	9.111938	-11.934271	-10.665760	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
218	2	9.457296	-13.145309	-10.052253	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
219	2	9.798434	-11.548607	-11.824853	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
220	2	10.463020	-13.953231	-10.582683	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
221	2	10.804494	-12.356074	-12.357267	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
222	2	11.138235	-13.559299	-11.736853	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
223	2	6.179934	-5.947943	-1.504465	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
224	2	7.226118	-6.875006	-1.597975	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
225	2	6.112309	-5.133600	-0.364807	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
226	2	8.170085	-6.992484	-0.579052	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
227	2	7.062465	-5.243596	0.650271	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
228	2	8.089914	-6.177612	0.546870	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
229	2	7.847289	-11.582089	-6.050557	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
230	2	8.656569	-10.491498	-6.401414	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
231	2	8.410527	-12.865871	-6.074051	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
232	2	9.990343	-10.679932	-6.764325	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
233	2	9.744282	-13.055151	-6.436633	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
234	2	10.535915	-11.962035	-6.784206	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
235	2	-14.101235	2.078016	-6.231150	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
236	2	-14.158669	1.818742	-4.855119	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
237	2	-15.109302	2.862668	-6.807911	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
238	2	-15.192549	2.333795	-4.072987	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
239	2	-16.148149	3.373041	-6.028195	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
240	2	-16.191105	3.108791	-4.660106	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
241	2	-9.116120	-0.441671	-0.657780	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
242	2	-10.082244	-0.294425	0.346811	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
243	2	-8.161289	0.568983	-0.822570	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
244	2	-10.091271	0.836232	1.165751	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
245	2	-8.177003	1.704099	-0.014712	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
246	2	-9.139586	1.839044	0.984591	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0



247	2	-2.287700	-5.668473	-2.335412	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
248	2	-1.809266	-6.816739	-1.692790	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
249	2	-1.577654	-5.159599	-3.430361	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
250	2	-0.647669	-7.446668	-2.138369	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
251	2	-0.415928	-5.786936	-3.873641	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
252	2	0.046807	-6.933297	-3.233094	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
253	2	-5.894035	0.007175	-4.117218	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
254	2	-4.915627	0.577324	-3.294902	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
255	2	-5.676023	-1.279084	-4.629548	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
256	2	-3.739092	-0.114491	-3.010347	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
257	2	-4.501059	-1.973164	-4.341305	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
258	2	-3.528111	-1.388033	-3.533786	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
259	3	-2.104324	2.351105	-5.388050	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
260	2	-2.881431	3.375466	-4.596669	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
261	2	-4.267224	3.473158	-4.761856	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
262	2	-2.248699	4.240608	-3.695271	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
263	2	-5.018801	4.397957	-4.039372	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
264	2	-2.984446	5.181546	-2.967459	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
265	2	-4.367024	5.258312	-3.152611	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
266	16	-2.426692	6.082134	-2.101544	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
267	16	-6.366355	4.385798	-4.263089	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
268	3	-1.295160	5.746654	-1.301446	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
269	3	-7.230601	5.145552	-3.432688	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
270	2	-8.644228	4.873607	-3.886670	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
271	2	-9.129311	5.466562	-5.057215	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
272	2	-9.501835	4.057564	-3.138859	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
273	2	-10.449661	5.281489	-5.466516	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
274	2	-10.831711	3.868062	-3.529775	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
275	2	-11.296540	4.487399	-4.690234	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
276	2	-1.772131	5.192428	0.020453	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
277	2	-1.792730	5.996538	1.165475	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
278	2	-2.194160	3.862962	0.128562	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
279	2	-2.213815	5.495868	2.398677	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
280	2	-2.640885	3.344467	1.350617	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
281	2	-2.645784	4.168790	2.481618	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
282	16	-10.832534	5.924199	-6.610978	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
283	16	-11.748850	3.132128	-2.833293	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
284	16	-2.164800	6.373285	3.447913	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
285	16	-3.090129	2.059222	1.506341	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
286	3	-12.212132	6.134547	-6.880678	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
287	3	-2.116558	5.921376	4.796525	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
288	3	-3.158756	1.212268	0.367479	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
289	3	-11.330738	2.242197	-1.809955	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
290	2	-12.849907	6.954910	-5.782741	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
291	2	-14.131829	6.643580	-5.313831	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
292	2	-12.165981	8.028508	-5.196364	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
293	2	-14.714826	7.382575	-4.285419	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
294	2	-12.732877	8.766870	-4.156818	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
295	2	-14.021986	8.453011	-3.719592	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
296	2	-12.565868	1.817121	-1.054228	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
297	2	-13.065778	2.654245	-0.049750	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
298	2	-13.219225	0.607853	-1.320588	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
299	2	-14.191268	2.296520	0.693802	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
300	2	-14.360580	0.244056	-0.599281	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
301	2	-14.828512	1.088922	0.408863	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
302	2	-3.487267	5.624410	5.357499	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
303	2	-3.644746	4.648368	6.349531	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
304	2	-4.621217	6.315845	4.914074	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
305	2	-4.901834	4.346085	6.873995	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
306	2	-5.888427	6.024631	5.428362	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
307	2	-6.018600	5.045251	6.412767	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
308	2	-3.697297	-0.140587	0.769561	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
309	2	-5.034227	-0.283540	1.155533	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
310	2	-2.888728	-1.284107	0.717086	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
311	2	-5.564304	-1.532681	1.482343	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
312	2	-3.399415	-2.543290	1.048830	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
313	2	-4.739062	-2.656708	1.423454	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0

314	16	-15.962714	7.045236	-3.852400	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
315	16	-11.980690	9.771939	-3.616445	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
316	16	-14.731955	3.058670	1.692820	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
317	16	-15.084456	-0.895742	-0.812391	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
318	16	-4.962763	3.343618	7.801815	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
319	16	-7.048148	6.609607	4.999064	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
320	16	-6.882576	-1.564082	1.842409	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
321	16	-2.697339	-3.716107	1.004266	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	0	0
322	3	-11.953464	9.945286	-2.202131	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
323	3	-16.002068	6.276426	-2.654924	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
324	3	-14.260652	4.375558	1.952520	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
325	3	-14.840125	-1.727550	-1.938856	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
326	3	-6.165143	2.595928	7.947533	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
327	3	-7.594933	-2.786180	1.981082	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
328	3	-7.083702	7.305591	3.759944	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
329	3	-1.284105	-3.779600	0.854564	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	0	0
330	2	-10.986126	8.982722	-1.546656	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
331	2	-11.133843	7.593775	-1.664611	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
332	2	-9.923222	9.470902	-0.771615	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
333	2	-10.255764	6.721175	-1.023074	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
334	2	-9.037816	8.598417	-0.136329	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
335	2	-9.203378	7.220391	-0.260053	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
336	2	-15.730125	7.157850	-1.459220	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
337	2	-14.529674	7.053519	-0.745767	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
338	2	-16.673618	8.110543	-1.053249	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
339	2	-14.271189	7.890635	0.340060	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
340	2	-16.419790	8.943460	0.036869	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
341	2	-15.216881	8.835935	0.733517	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
342	2	-12.924502	4.360447	2.659235	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
343	2	-11.858684	5.154859	2.212516	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
344	2	-12.736655	3.569363	3.800196	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
345	2	-10.635489	5.151269	2.882936	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
346	2	-11.516132	3.570693	4.475963	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
347	2	-10.462878	4.360903	4.017682	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
348	2	-13.673909	-2.665003	-1.723521	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
349	2	-13.097843	-3.303691	-2.830503	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
350	2	-13.172876	-2.958407	-0.447222	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
351	2	-12.053452	-4.213367	-2.667404	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
352	2	-12.124055	-3.864429	-0.283249	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
353	2	-11.564492	-4.496075	-1.393037	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
354	2	-6.594276	2.003345	6.624148	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
355	2	-5.648852	1.432570	5.762220	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
356	2	-7.938845	2.020094	6.227360	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
357	2	-6.030610	0.913856	4.526354	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
358	2	-8.323031	1.490918	4.994429	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
359	2	-7.368674	0.944329	4.139922	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
360	2	-0.628018	-3.738828	2.213107	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
361	2	-0.355829	-2.525060	2.856673	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
362	2	-0.250487	-4.932366	2.845906	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
363	2	0.278241	-2.504977	4.097424	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
364	2	0.378461	-4.913206	4.090401	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
365	2	0.642821	-3.697330	4.715653	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
366	2	-7.175780	-3.581733	3.196247	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
367	2	-6.615121	-2.974081	4.327818	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
368	2	-7.356886	-4.972549	3.205915	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
369	2	-6.229827	-3.735587	5.430960	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
370	2	-6.977680	-5.735094	4.311311	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
371	2	-6.408987	-5.117652	5.423934	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
372	2	-6.578197	6.453809	2.616969	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	0	0
373	2	-6.699739	5.057014	2.623984	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
374	2	-5.928607	7.062389	1.533953	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
375	2	-6.168018	4.290582	1.589375	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
376	2	-5.413852	6.296565	0.488715	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
377	2	-5.532994	4.908487	0.514238	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	0	0
378	41	0.780804	-3.022229	-5.708659	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
379	41	-1.104605	0.629779	-6.976449	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
380	41	0.607305	-0.410250	-0.517939	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0

381	41	2.136487	-6.324157	-0.749312	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
382	41	1.306854	-4.649017	-2.311232	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
383	41	2.833771	-3.238417	2.196687	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
384	41	2.008280	-1.540276	0.627890	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
385	41	1.806567	-7.401902	1.928500	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
386	41	3.016242	-7.505886	0.606506	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
387	41	5.461545	-7.594923	1.112117	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
388	41	2.448978	-8.317554	4.111788	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
389	41	6.485306	-9.751164	4.708479	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
390	41	2.135788	-9.958789	5.701446	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
391	41	2.910507	-10.233706	7.272650	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
392	41	8.730973	-9.418230	3.731714	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
393	41	7.844954	-10.740588	2.881712	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
394	41	10.856500	-8.636773	2.759950	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
395	41	8.089117	-10.905470	0.354443	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
396	41	11.958640	-9.883152	-1.232274	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
397	41	0.745422	-8.945560	7.884487	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
398	41	4.163599	-7.094419	6.016306	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
399	41	1.287391	-7.667320	8.120014	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
400	41	14.248724	-7.336285	0.248348	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
401	41	13.700222	-8.612688	-0.853029	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
402	41	-1.307674	-8.325165	8.244668	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
403	41	-2.182566	-7.159881	9.259826	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
404	41	5.280730	-4.985020	5.807156	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
405	41	3.862217	-5.295597	4.739663	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
406	41	8.095966	-9.821821	-2.247872	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
407	41	8.547910	-11.023601	-3.474399	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
408	41	12.227796	-7.883259	-2.640281	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
409	41	12.325203	-5.643859	1.050367	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
410	41	9.852356	-4.304042	-2.214217	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
411	41	5.933522	-10.426494	-1.394214	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
412	41	8.837232	-13.523112	-2.128793	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
413	41	5.066423	-14.509047	-0.262949	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
414	41	-1.722863	-4.569341	8.127314	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
415	41	-2.364884	-8.306396	6.060078	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
416	41	-3.347013	-4.553070	4.142602	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
417	41	5.343813	-4.098576	3.112298	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
418	41	3.464541	-2.086583	6.448509	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
419	41	4.721800	0.158322	2.987815	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
420	41	10.601789	-4.478374	2.112630	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
421	41	11.944936	-3.369241	1.652328	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
422	41	8.690131	-5.452303	-3.840223	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
423	41	10.032305	-4.499989	-4.578516	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
424	41	4.882374	-10.719419	1.122833	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
425	41	4.034884	-10.024887	-0.300268	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
426	41	8.763000	-16.871769	-0.472960	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
427	41	9.345866	-15.598890	-1.562220	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
428	41	-2.520284	-2.225398	7.937764	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
429	41	-0.928492	-2.650931	7.199535	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
430	41	4.488144	-0.456870	0.843275	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
431	41	6.235389	-0.110219	1.098573	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
432	41	-4.632674	-5.994654	2.935894	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
433	41	-2.933214	-5.959019	2.342762	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
434	41	3.298466	2.297645	5.624841	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
435	41	4.707649	1.806217	4.664341	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
436	41	8.941332	-3.514290	3.507303	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
437	41	10.993610	-0.983837	0.649137	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
438	41	7.665356	-1.549476	4.325816	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
439	41	9.699920	0.977925	1.467671	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
440	41	8.034813	0.701977	3.312831	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
441	41	11.335147	-6.428949	-6.395227	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
442	41	7.116827	-5.832551	-5.590496	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
443	41	10.771441	-7.322439	-8.646470	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
444	41	6.567055	-6.724995	-7.834514	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
445	41	8.386600	-7.474212	-9.375813	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
446	41	3.535702	-12.089186	2.818579	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
447	41	1.633471	-9.662675	-0.217796	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0

448	41	1.417819	-12.103240	4.124530	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
449	41	-0.473763	-9.670349	1.090170	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
450	41	-0.593184	-10.888825	3.270752	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
451	41	7.558311	-15.810063	1.804477	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
452	41	10.776509	-13.995622	-0.462443	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
453	41	8.238742	-14.497687	3.805408	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
454	41	11.441019	-12.685349	1.535106	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
455	41	10.180977	-12.928158	3.676361	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
456	41	-3.007897	-1.149850	4.653466	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
457	41	-0.523164	-0.212108	8.085457	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
458	41	-2.663320	1.137968	3.789009	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
459	41	-0.185617	2.086869	7.200362	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
460	41	-1.241215	2.762841	5.038733	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
461	41	1.073244	0.682759	4.457253	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
462	41	4.290126	2.833387	2.512468	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
463	41	-0.342630	0.982362	2.435329	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
464	41	2.869703	3.121454	0.493850	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
465	41	0.547199	2.205700	0.448485	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
466	41	7.833737	-1.963027	-0.195495	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
467	41	3.819542	-0.834795	-1.369852	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
468	41	8.293461	-2.708625	-2.521668	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
469	41	4.281096	-1.593139	-3.684967	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
470	41	6.522127	-2.538543	-4.275602	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
471	41	-5.558077	-6.354923	0.704989	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
472	41	-2.649279	-9.126962	2.328710	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
473	41	-6.079145	-7.968976	-1.108570	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
474	41	-3.182295	-10.740434	0.512711	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
475	41	-4.894710	-10.166735	-1.213792	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
476	41	0.169856	-2.879761	-9.366199	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
477	41	1.179997	-3.112446	-7.925909	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
478	41	0.687006	-5.456238	-7.527540	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
479	41	-2.574426	-2.686391	-8.042007	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
480	41	-3.365055	-6.711778	-6.696226	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
481	41	-4.698049	-2.428913	-7.447220	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
482	41	-4.715788	-3.310230	-9.018560	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
483	41	-1.840827	-8.285105	-5.239957	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
484	41	-2.356770	-8.716619	-6.910815	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
485	41	-0.706543	-9.953832	-8.424128	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
486	41	-0.198702	-9.733032	-4.142357	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
487	41	1.871851	-12.768769	-6.400723	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
488	41	-6.765366	-2.163577	-9.678965	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
489	41	-6.673942	-4.587488	-6.117599	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
490	41	-10.458467	-3.284581	-7.750500	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
491	41	2.269644	-13.427945	-8.409073	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
492	41	2.066731	-12.969044	-10.107174	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
493	41	-8.098628	-0.487939	-10.377069	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
494	41	-9.816249	-0.160477	-10.682822	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
495	41	-9.678408	-6.154632	-4.487780	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
496	41	-8.319030	-6.395901	-5.603616	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
497	41	1.014511	-10.511215	-2.550648	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
498	41	2.220310	-11.741759	-2.133224	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
499	41	4.647689	-13.122568	-9.872664	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
500	41	2.311016	-9.917610	-8.166735	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
501	41	6.501165	-9.341290	-8.895872	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
502	41	2.330543	-8.504927	-2.061558	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
503	41	4.028868	-11.581538	-4.564912	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
504	41	6.003427	-7.774566	-4.207616	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
505	41	-11.362516	0.448478	-8.788018	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
506	41	-7.112481	0.011792	-8.165673	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
507	41	-9.527622	1.959695	-5.176126	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
508	41	-6.341780	-6.429491	-4.296975	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
509	41	-9.343649	-3.464234	-3.390319	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
510	41	-5.576369	-3.429200	-1.286459	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
511	41	2.372733	-7.711340	-8.204203	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
512	41	2.862877	-8.282231	-6.564200	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
513	41	7.831117	-10.187053	-10.727497	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
514	41	8.358209	-10.691184	-9.082915	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0

515	41	5.623993	-5.803262	-3.609919	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
516	41	4.696099	-4.773257	-2.520332	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
517	41	6.213536	-12.092387	-4.759854	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
518	41	5.171839	-11.688812	-6.446088	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
519	41	-12.972449	1.986224	-8.077976	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
520	41	-13.149266	0.415523	-7.206660	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
521	41	-3.500836	-3.909184	-2.061231	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
522	41	-3.772228	-5.184076	-0.820037	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
523	41	-7.293849	1.664637	-3.865527	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
524	41	-8.034703	0.082183	-4.283305	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
525	41	-9.294637	-1.313759	-2.613139	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
526	41	-9.887128	-2.367792	-1.278771	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
527	41	4.162342	-5.666885	-9.017457	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
528	41	2.737335	-6.493083	-5.014092	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
529	41	4.543440	-3.290688	-8.387672	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
530	41	3.109768	-4.114206	-4.392418	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
531	41	4.015623	-2.503909	-6.077415	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
532	41	8.927621	-13.465701	-9.139495	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
533	41	9.547298	-10.599422	-12.326828	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
534	41	10.722888	-14.904189	-10.088403	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
535	41	11.337150	-12.042069	-13.270728	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
536	41	11.933149	-14.197419	-12.157882	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
537	41	7.324321	-7.519844	-2.483705	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
538	41	5.307173	-4.385719	-0.265099	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
539	41	8.991556	-7.722466	-0.667456	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
540	41	7.002901	-4.588269	1.533882	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
541	41	8.840813	-6.271217	1.348088	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
542	41	8.248121	-9.466764	-6.390087	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
543	41	7.797234	-13.740234	-5.798122	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
544	41	10.613637	-9.811290	-7.035137	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
545	41	10.173512	-14.071062	-6.449678	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
546	41	11.589458	-12.110455	-7.074701	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
547	41	-13.376182	1.204361	-4.379684	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
548	41	-15.091626	3.079242	-7.889145	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
549	41	-15.220239	2.126288	-2.989666	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
550	41	-16.937559	3.986637	-6.494378	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
551	41	-17.013111	3.510004	-4.044403	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
552	41	-10.851478	-1.070978	0.494051	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
553	41	-7.385780	0.468027	-1.598791	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
554	41	-10.860710	0.944572	1.949530	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
555	41	-7.426512	2.494456	-0.173331	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
556	41	-9.153641	2.736459	1.626317	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
557	41	-2.361269	-7.238335	-0.835971	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
558	41	-1.943715	-4.266142	-3.963311	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
559	41	-0.288955	-8.355421	-1.628457	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
560	41	0.132771	-5.379977	-4.738248	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
561	41	0.957252	-1.429525	-3.603216	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
562	41	-5.064688	1.585236	-2.873654	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
563	41	-6.440129	-1.749129	-5.271597	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
564	41	-2.969388	0.351348	-2.375970	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
565	41	-4.343618	-2.984446	-4.752451	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
566	41	-2.595059	-1.928970	-3.308723	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
567	41	-1.552000	2.846791	-6.214647	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
568	41	-2.807256	1.609704	-5.825345	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
569	41	-4.786332	2.803830	-5.468563	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
570	41	-1.155368	4.177939	-3.585443	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
571	41	-4.930687	6.014050	-2.586582	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
572	41	-0.611230	5.039361	-1.809518	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
573	41	-0.703737	6.671256	-1.131590	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
574	41	-7.097009	4.854887	-2.368575	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
575	41	-7.007797	6.229961	-3.526735	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1 H 0
576	41	-8.466157	6.107716	-5.661397	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
577	41	-9.113680	3.589897	-2.222060	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
578	41	-12.345875	4.328972	-4.980850	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
579	41	-1.463371	7.046810	1.103970	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
580	41	-2.176077	3.237905	-0.777538	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
581	41	-3.013036	3.760748	3.435616	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0

582	41	-12.303011	6.684039	-7.841949	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
583	41	-12.723423	5.160507	-7.029851	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
584	41	-1.434083	5.050487	4.880278	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
585	41	-1.661423	6.727797	5.411168	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
586	41	-3.831043	1.658719	-0.396903	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
587	41	-2.148312	1.098499	-0.078213	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
588	41	-10.801495	1.373882	-2.255544	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
589	41	-10.641519	2.750942	-1.106671	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
590	41	-14.690637	5.801134	-5.751591	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
591	41	-11.150548	8.287681	-5.539386	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
592	41	-14.505369	9.045232	-2.928412	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
593	41	-12.544013	3.601334	0.148549	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
594	41	-12.820347	-0.050972	-2.107285	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
595	41	-15.724654	0.802514	0.983266	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
596	41	-2.769136	4.090081	6.718301	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
597	41	-4.501144	7.087848	4.138969	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
598	41	-7.022989	4.824174	6.803443	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
599	41	-5.689322	0.602087	1.192880	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
600	41	-1.844053	-1.173510	0.393860	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
601	41	-5.129943	-3.653470	1.674976	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
602	41	-11.637497	10.990340	-1.997450	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
603	41	-12.962762	9.847192	-1.755052	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
604	41	-17.011448	5.822958	-2.557151	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
605	41	-15.283042	5.431537	-2.715885	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
606	41	-14.232667	4.960130	1.011333	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
607	41	-14.999582	4.886043	2.606903	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
608	41	-15.749249	-2.344144	-2.109086	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
609	41	-14.713386	-1.111078	-2.853852	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
610	41	-5.983172	1.773577	8.672052	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
611	41	-6.956145	3.234432	8.393544	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
612	41	-8.675752	-2.545930	2.075827	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
613	41	-7.490356	-3.385921	1.052247	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
614	41	-8.134212	7.602350	3.553645	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
615	41	-6.504226	8.248934	3.850249	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
616	41	-1.033377	-4.737615	0.352209	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
617	41	-0.910521	-2.985748	0.180934	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	O
618	41	-11.951350	7.171981	-2.270495	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
619	41	-9.778321	10.558042	-0.655919	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
620	41	-10.396393	5.633074	-1.121894	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
621	41	-8.207067	9.000211	0.467053	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
622	41	-8.506941	6.527553	0.241110	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
623	41	-13.774346	6.310789	-1.051471	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
624	41	-17.623695	8.211832	-1.604685	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
625	41	-13.315764	7.809999	0.884873	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
626	41	-17.169514	9.691747	0.344054	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
627	41	-15.013061	9.498226	1.591553	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
628	41	-11.978465	5.794616	1.322683	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
629	41	-13.562859	2.941839	4.174970	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
630	41	-9.806090	5.779570	2.517794	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
631	41	-11.387573	2.948351	5.377164	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
632	41	-9.498291	4.364671	4.552709	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
633	41	-13.480573	-3.099746	-3.844906	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
634	41	-13.612657	-2.481360	0.444906	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
635	41	-11.620607	-4.714707	-3.548931	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
636	41	-11.743080	-4.087487	0.727734	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
637	41	-10.739797	-5.217224	-1.262762	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
638	41	-4.586323	1.402417	6.055555	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
639	41	-8.705265	2.456517	6.889024	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
640	41	-5.271179	0.477830	3.856956	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
641	41	-9.382140	1.504204	4.689186	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
642	41	-7.673272	0.532588	3.163961	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
643	41	-0.635263	-1.570159	2.386086	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
644	41	-0.446584	-5.902232	2.360453	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
645	41	0.489977	-1.545074	4.594843	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
646	41	0.664854	-5.857909	4.582376	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
647	41	1.136162	-3.675136	5.699224	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O
648	41	-6.466189	-1.882365	4.354546	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	O



649	41	-7.802856	-5.476882	2.332247	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
650	41	-5.778425	-3.242269	6.308374	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
651	41	-7.120469	-6.828881	4.303203	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
652	41	-6.097791	-5.719493	6.294339	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
653	41	-7.188457	4.542149	3.468122	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
654	41	-5.805216	8.157759	1.507362	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
655	41	-6.233324	3.191712	1.639977	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
656	41	-4.890347	6.790412	-0.346105	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0
657	41	-5.104856	4.300809	-0.299815	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1 H 0

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1	2	49.764347	-35.543568	0.424984	1 " " X " "	2	0.00000	0.00000	" " " C " " "	6	0	0	1 C 0
2	2	50.632629	-36.319141	1.209755	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
3	2	48.667114	-34.907810	1.040236	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
4	2	50.405884	-36.455009	2.580081	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
5	2	48.461704	-35.054195	2.418691	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
6	2	49.322205	-35.833179	3.194570	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
7	2	50.030884	-35.440319	-0.948461	1 " " X " "	2	0.32058	0.32058	" " " C " " "	6	0	0	1 C 0
8	2	51.137600	-36.112244	-1.457929	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
9	16	51.719261	-36.983036	0.711564	1 " " X " "	70	-0.00030	-0.00030	" " " O " " "	8	0	0	1 O 0
10	2	51.962448	-36.872341	-0.627845	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
11	2	55.019779	-37.778175	-2.674515	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
12	2	55.387978	-39.003094	-2.115071	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
13	2	53.907520	-37.080933	-2.200009	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
14	2	54.622742	-39.521309	-1.066385	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
15	2	53.135754	-37.595009	-1.151305	1 " " X " "	2	0.00000	0.00000	" " " C " " "	6	0	0	1 C 0
16	2	53.512169	-38.821136	-0.589985	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
17	15	49.333664	-34.791389	-1.696725	1 " " X " "	70	-0.32058	-0.32058	" " " O " " "	8	0	0	1 O 0
18	16	47.815517	-34.174690	0.257006	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
19	16	49.169437	-36.050690	4.535458	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
20	16	56.493191	-39.612095	-2.639991	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
21	3	49.749969	-32.935619	-6.580737	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
22	2	49.430531	-33.089111	-8.051105	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
23	2	48.549976	-32.203526	-8.685862	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
24	2	49.987549	-34.132366	-8.801969	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
25	2	48.195663	-32.372898	-10.023765	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
26	2	49.658314	-34.310669	-10.147867	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
27	2	48.749691	-33.433044	-10.744491	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
28	16	47.301533	-31.479740	-10.546773	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
29	16	50.258423	-35.355873	-10.798549	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
30	3	46.948753	-31.557381	-11.922481	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
31	3	49.801514	-35.814770	-12.067605	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
32	2	45.942570	-30.468266	-12.205874	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
33	2	46.286774	-29.120918	-12.055957	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
34	2	44.653187	-30.781872	-12.647810	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
35	2	45.372684	-28.104319	-12.340105	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
36	2	43.723328	-29.782202	-12.936410	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
37	2	44.087112	-28.441000	-12.777553	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
38	2	50.089046	-34.820076	-13.169086	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
39	2	49.068619	-34.429104	-14.044567	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
40	2	51.365662	-34.267262	-13.335262	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
41	2	49.306854	-33.495907	-15.051297	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
42	2	51.618443	-33.326763	-14.341671	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1 C 0
43	2	50.578487	-32.941669	-15.191776	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
44	16	45.827389	-26.824913	-12.176318	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
45	16	42.503185	-30.208220	-13.380771	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
46	16	48.283485	-33.098164	-15.859170	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
47	16	52.833988	-32.735329	-14.551874	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1 O 0
48	3	45.073753	-25.705574	-12.625968	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
49	3	48.164337	-33.786915	-17.098417	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
50	3	41.503616	-29.277826	-13.773975	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
51	3	53.979134	-33.196545	-13.845580	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1 C 0
52	2	43.911781	-25.403051	-11.708660	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1 C 0
53	2	42.726307	-24.872059	-12.234979	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
54	2	43.996849	-25.612959	-10.325370	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0
55	2	41.651691	-24.564533	-11.401262	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1 C 0

56	2	42.920658	-25.308634	-9.491164	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
57	2	41.745258	-24.785587	-10.028234	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
58	2	55.168144	-32.373592	-14.283455	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
59	2	55.525455	-32.301201	-15.636416	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
60	2	55.949409	-31.684448	-13.345193	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
61	2	56.635906	-31.560633	-16.042698	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
62	2	57.059505	-30.942179	-13.750364	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
63	2	57.404850	-30.880156	-15.099659	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
64	2	47.707058	-35.210701	-16.880869	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
65	2	48.404476	-36.284939	-17.449083	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
66	2	46.566471	-35.483128	-16.113001	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
67	2	47.980160	-37.598282	-17.244465	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
68	2	46.142662	-36.795841	-15.905003	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
69	2	46.849522	-37.855728	-16.470551	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
70	2	40.352871	-30.060211	-14.362699	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
71	2	39.833344	-29.740782	-15.624638	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
72	2	39.776749	-31.120445	-13.650898	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
73	2	38.763824	-30.460945	-16.158052	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
74	2	38.707523	-31.841602	-14.182291	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
75	2	38.198837	-31.512022	-15.437249	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
76	3	45.757343	-30.008255	-4.190013	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
77	2	46.034760	-31.201345	-5.077533	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
78	2	47.271667	-31.855875	-5.026320	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
79	2	45.066093	-31.670223	-5.975982	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
80	2	47.521885	-32.965374	-5.832405	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
81	2	45.302601	-32.781540	-6.789665	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
82	2	46.532379	-33.440765	-6.693121	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
83	16	44.308319	-33.141560	-7.660026	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
84	16	48.740410	-33.576206	-5.804155	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
85	3	44.558361	-34.175350	-8.605585	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
86	2	43.409500	-34.247417	-9.585121	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
87	2	43.660141	-34.213081	-10.963331	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
88	2	42.084854	-34.381958	-9.149349	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
89	2	42.624481	-34.303200	-11.895263	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
90	2	41.036514	-34.468788	-10.070568	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
91	2	41.310474	-34.435665	-11.439045	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
92	16	42.984360	-34.261013	-13.213830	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
93	16	39.734524	-34.623253	-9.688715	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
94	3	41.990078	-34.214603	-14.229112	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
95	3	39.188644	-33.685162	-8.768401	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
96	2	42.708424	-34.085915	-15.550936	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
97	2	42.831181	-35.172993	-16.423365	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
98	2	43.276203	-32.862892	-15.924277	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
99	2	43.514801	-35.052406	-17.635399	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
100	2	43.947407	-32.716625	-17.138777	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
101	2	44.067600	-33.818439	-17.990952	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
102	2	39.049725	-32.343475	-9.449540	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
103	2	40.080196	-31.399940	-9.378817	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
104	2	37.893818	-32.021095	-10.169513	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
105	2	39.962036	-30.151667	-9.994901	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
106	2	37.761505	-30.785498	-10.806401	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
107	2	38.799774	-29.853752	-10.709640	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
108	16	43.611340	-36.184429	-18.396355	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
109	16	44.467915	-31.480244	-17.402435	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
110	16	40.932171	-29.187351	-9.960497	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
111	16	36.602749	-30.577230	-11.501487	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
112	3	44.662876	-36.332882	-19.345261	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
113	3	41.980793	-29.235931	-8.998281	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
114	3	44.674011	-31.053568	-18.743542	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
115	3	36.433716	-29.393055	-12.270929	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
116	2	44.338562	-35.658398	-20.658043	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
117	2	43.047863	-35.705521	-21.201754	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
118	2	45.344357	-34.992672	-21.373205	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
119	2	42.767139	-35.095753	-22.424995	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
120	2	45.065079	-34.384304	-22.597399	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
121	2	43.775486	-34.434467	-23.124687	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
122	2	35.117985	-29.507864	-13.004473	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0



123	2	35.067101	-29.438467	-14.403105	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
124	2	33.920948	-29.681633	-12.297001	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
125	2	33.850060	-29.538794	-15.077844	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
126	2	32.703930	-29.786236	-12.970630	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
127	2	32.666348	-29.712898	-14.362176	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
128	2	41.411808	-29.003643	-7.616126	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
129	2	41.435219	-29.998344	-6.628601	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
130	2	40.837223	-27.764679	-7.302091	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
131	2	40.885483	-29.765039	-5.367776	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
132	2	40.288738	-27.528730	-6.041405	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
133	2	40.309700	-28.530575	-5.072639	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
134	2	43.345322	-30.917690	-19.450472	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
135	2	43.101124	-31.576143	-20.662485	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
136	2	42.331371	-30.118391	-18.904339	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
137	2	41.871960	-31.445864	-21.309540	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
138	2	41.101894	-29.986477	-19.550611	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
139	2	40.870190	-30.651104	-20.754072	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
140	3	37.583008	-37.056168	-0.775571	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
141	2	36.583385	-35.980778	-0.417535	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
142	2	35.344398	-35.891800	-1.062163	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
143	2	36.880795	-35.052307	0.586764	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
144	2	34.424686	-34.896698	-0.724252	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
145	2	35.981926	-34.041515	0.929899	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
146	2	34.752934	-33.967239	0.268318	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
147	16	33.239925	-34.904419	-1.406960	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
148	16	36.388042	-33.180946	1.911795	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
149	3	32.167011	-34.072590	-0.983465	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
150	3	35.787819	-31.899982	2.059760	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
151	2	30.928391	-34.423473	-1.776477	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
152	2	30.671057	-35.727810	-2.217342	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
153	2	29.984186	-33.430679	-2.060872	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
154	2	29.507734	-36.038193	-2.926050	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
155	2	28.811142	-33.720535	-2.758326	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
156	2	28.576374	-35.028996	-3.186477	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
157	2	34.474216	-31.974380	2.801994	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
158	2	33.361500	-31.266403	2.335474	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
159	2	34.350231	-32.701866	3.991249	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
160	2	32.146740	-31.287407	3.019737	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
161	2	33.148865	-32.721050	4.704134	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
162	2	32.045982	-32.017849	4.206604	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
163	16	29.362057	-37.339970	-3.322058	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
164	16	27.952745	-32.679600	-2.972837	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
165	16	31.132120	-30.555231	2.467863	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
166	16	33.140892	-33.418560	5.881563	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
167	3	28.204674	-37.784534	-4.021264	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
168	3	29.820417	-30.558874	3.017204	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
169	3	26.745733	-32.870033	-3.700062	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
170	3	32.022495	-33.306801	6.753621	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
171	2	28.111109	-37.172604	-5.401023	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
172	2	29.244888	-37.032757	-6.213107	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
173	2	26.873457	-36.737076	-5.896667	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
174	2	29.146500	-36.461349	-7.482371	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
175	2	26.774286	-36.165371	-7.165300	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
176	2	27.911020	-36.026314	-7.959675	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
177	2	32.373478	-33.977753	8.060281	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
178	2	32.507568	-35.370197	8.136025	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
179	2	32.556313	-33.220341	9.225733	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
180	2	32.813663	-35.990944	9.347754	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
181	2	32.857357	-33.840561	10.438479	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
182	2	32.984879	-35.226959	10.501573	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
183	2	29.156174	-31.902592	2.823573	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
184	2	29.259567	-32.586143	1.604525	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
185	2	28.402681	-32.479725	3.855028	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
186	2	28.633265	-33.819393	1.422557	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
187	2	27.776794	-33.713562	3.674781	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
188	2	27.891935	-34.385284	2.458542	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
189	2	26.056665	-31.527122	-3.741956	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0

190	2	25.399696	-31.035885	-2.605995	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
191	2	26.072206	-30.742912	-4.902874	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
192	2	24.784365	-29.784124	-2.624317	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
193	2	25.456388	-29.491091	-4.922757	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
194	2	24.813883	-29.009169	-3.782863	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
195	3	46.705635	-33.474602	0.806093	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
196	2	45.902153	-32.932758	-0.351966	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
197	2	44.692001	-33.532104	-0.719742	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
198	2	46.354305	-31.831236	-1.087768	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
199	2	43.939602	-33.044205	-1.788727	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
200	2	45.622883	-31.338545	-2.170898	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
201	2	44.408794	-31.943123	-2.510100	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
202	16	46.160706	-30.280725	-2.851435	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
203	16	42.771957	-33.699329	-2.061547	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
204	3	41.870342	-33.180534	-3.029943	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
205	2	40.623722	-34.034111	-3.067042	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
206	2	40.265438	-34.887775	-2.014884	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
207	2	39.780304	-33.964504	-4.182838	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
208	2	39.102554	-35.659550	-2.066836	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
209	2	38.608055	-34.717537	-4.244500	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
210	2	38.275925	-35.571293	-3.189889	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
211	16	37.842712	-34.613869	-5.369112	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
212	16	38.864212	-36.476704	-0.995684	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
213	3	36.452255	-34.359394	-5.207123	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
214	2	36.246906	-32.920872	-4.793316	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
215	2	35.730347	-32.590137	-3.534640	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
216	2	36.534237	-31.889849	-5.696607	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
217	2	35.490196	-31.261377	-3.177145	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
218	2	36.300495	-30.554592	-5.356877	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
219	2	35.793617	-30.249701	-4.093048	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
220	16	34.945732	-31.040810	-1.940179	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
221	16	36.489445	-29.494341	-6.198547	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
222	3	34.254429	-29.835148	-1.618567	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
223	3	36.842148	-29.702194	-7.560872	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
224	2	32.814354	-29.872850	-2.086967	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
225	2	31.769604	-29.617096	-1.187434	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
226	2	32.478355	-30.136127	-3.420501	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
227	2	30.433937	-29.628199	-1.597247	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
228	2	31.152193	-30.155554	-3.851620	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
229	2	30.129337	-29.897268	-2.935590	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
230	2	36.389400	-28.482092	-8.325404	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
231	2	35.045250	-28.345467	-8.691319	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
232	2	37.291271	-27.483706	-8.703914	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
233	2	34.605484	-27.244751	-9.427457	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
234	2	36.873035	-26.374760	-9.440772	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
235	2	35.525677	-26.259300	-9.797332	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
236	16	29.494743	-29.373022	-0.635837	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
237	16	30.954988	-30.433050	-5.175389	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
238	16	33.276825	-27.215492	-9.749174	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
239	16	37.837029	-25.462328	-9.770175	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
240	3	28.111616	-29.464392	-0.953498	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
241	3	32.781132	-26.224907	-10.640727	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
242	3	29.639565	-30.594374	-5.686221	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
243	3	37.601807	-24.483044	-10.774943	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
244	2	27.332825	-29.180605	0.308187	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
245	2	26.687128	-30.211531	1.003616	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
246	2	27.243517	-27.874022	0.806057	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
247	2	25.974741	-29.944265	2.172861	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
248	2	26.530003	-27.605244	1.974665	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
249	2	25.895603	-28.640509	2.660225	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
250	2	37.441097	-25.142063	-12.125902	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
251	2	36.348038	-24.843327	-12.951234	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
252	2	38.396015	-26.060375	-12.583827	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
253	2	36.208485	-25.454308	-14.197941	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
254	2	38.261059	-26.664957	-13.833192	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
255	2	37.166264	-26.364782	-14.641450	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
256	2	31.308468	-26.491682	-10.841830	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0

257	2	30.407763	-26.335947	-9.779598	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
258	2	30.814753	-26.897490	-12.088811	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
259	2	29.046661	-26.586178	-9.957616	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
260	2	29.454088	-27.149286	-12.267680	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
261	2	28.568371	-26.994528	-11.202012	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
262	2	29.768061	-30.922447	-7.154122	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
263	2	30.136559	-29.928165	-8.070372	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
264	2	29.526253	-32.219421	-7.627266	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
265	2	30.261221	-30.222158	-9.428206	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
266	2	29.651239	-32.513515	-8.985818	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
267	2	30.018272	-31.515537	-9.887923	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
268	3	66.979385	-37.887699	-0.179030	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
269	2	66.998421	-38.035156	1.324813	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
270	2	68.185440	-38.380440	1.981283	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
271	2	65.851006	-37.812347	2.095625	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
272	2	68.229454	-38.497726	3.370334	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
273	2	65.872009	-37.954838	3.484849	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
274	2	67.068367	-38.299561	4.120019	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
275	16	69.436768	-38.790386	3.932213	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
276	16	64.693100	-37.731785	4.140744	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
277	3	69.772171	-38.149494	5.159715	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
278	3	64.475822	-38.257572	5.445307	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
279	2	71.278229	-38.064735	5.251297	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
280	2	72.051605	-37.884720	4.095967	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
281	2	71.923317	-38.135788	6.493521	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
282	2	73.443436	-37.795906	4.167745	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
283	2	73.314629	-38.026360	6.583047	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
284	2	74.060776	-37.861229	5.416033	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
285	2	64.978020	-37.363544	6.557696	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
286	2	65.687263	-36.174751	6.340763	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
287	2	64.696648	-37.738762	7.879566	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
288	2	66.116234	-35.380524	7.406524	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
289	2	65.103432	-36.948723	8.958333	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	C	0
290	2	65.816109	-35.774822	8.712600	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
291	16	74.260025	-37.648266	3.081322	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
292	16	74.025932	-38.059483	7.749319	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
293	16	66.796379	-34.238480	7.083845	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
294	16	64.834518	-37.234333	10.268416	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	O	0
295	3	73.721695	-37.757462	1.770426	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
296	3	67.280746	-33.356152	8.089774	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
297	3	73.378494	-38.240978	9.000482	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
298	3	64.099129	-38.401253	10.613269	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0
299	2	74.877609	-37.675350	0.802592	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
300	2	75.607109	-38.821651	0.460407	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
301	2	75.244034	-36.449928	0.231430	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
302	2	76.677498	-38.744682	-0.431473	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
303	2	76.313377	-36.372334	-0.661093	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
304	2	77.030655	-37.519787	-0.995272	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
305	2	63.875332	-38.390762	12.107547	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
306	2	64.944084	-38.192616	12.992427	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
307	2	62.592514	-38.587536	12.637911	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
308	2	64.734642	-38.181519	14.372076	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
309	2	62.383434	-38.581215	14.017331	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
310	2	63.453339	-38.374405	14.886520	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
311	2	68.470810	-33.949509	8.809053	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
312	2	68.568420	-33.897564	10.206542	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
313	2	69.515617	-34.541729	8.087303	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
314	2	69.676727	-34.433559	10.863990	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
315	2	70.626656	-35.072338	8.741968	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
316	2	70.708046	-35.021629	10.132721	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
317	2	74.375839	-38.062180	10.123199	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	C	0
318	2	73.929070	-38.157818	11.449064	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
319	2	75.733643	-37.794052	9.894027	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
320	2	74.812759	-37.990742	12.515758	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
321	2	76.618416	-37.627396	10.960114	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
322	2	76.159355	-37.725307	12.272631	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	C	0
323	3	62.999111	-41.636581	-2.992436	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	C	0

324	2	64.112991	-41.314846	-2.026755	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
325	2	64.446136	-39.981827	-1.766231	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
326	2	64.839355	-42.324810	-1.385778	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
327	2	65.485428	-39.653328	-0.896228	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
328	2	65.872482	-42.015747	-0.497962	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
329	2	66.192131	-40.676182	-0.258935	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
330	16	66.522079	-43.071301	0.081040	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
331	16	65.745575	-38.321789	-0.735825	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
332	3	67.420929	-42.879837	1.167779	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
333	2	68.775925	-42.347713	0.754199	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
334	2	69.702393	-42.023819	1.756240	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
335	2	69.153465	-42.173840	-0.584158	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
336	2	70.974854	-41.544216	1.433525	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
337	2	70.407684	-41.663174	-0.921720	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
338	2	71.316505	-41.360756	0.094115	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
339	16	71.943306	-41.247406	2.350359	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
340	16	70.681519	-41.514004	-2.252453	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
341	3	71.809158	-41.687275	3.695195	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
342	3	71.538635	-40.465286	-2.689869	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
343	2	73.124870	-41.524139	4.421186	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
344	2	73.150177	-41.615784	5.817710	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
345	2	74.334084	-41.308350	3.748187	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
346	2	74.344063	-41.495743	6.530442	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
347	2	75.537628	-41.168209	4.442542	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
348	2	75.536453	-41.264874	5.837348	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
349	2	70.835892	-39.138252	-2.522793	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
350	2	69.935883	-38.695621	-3.496834	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
351	2	71.073555	-38.317600	-1.415823	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
352	2	69.311462	-37.451145	-3.401731	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
353	2	70.431381	-37.086468	-1.279389	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
354	2	69.563881	-36.648548	-2.285532	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
355	16	74.256760	-41.629330	7.888091	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
356	16	76.654015	-40.961304	3.678642	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
357	16	68.501381	-37.105835	-4.448849	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
358	16	70.706100	-36.387383	-0.138001	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
359	3	75.436951	-41.742233	8.673470	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
360	3	67.911224	-35.815212	-4.565644	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
361	3	77.919594	-40.655365	4.253223	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
362	3	70.032112	-35.167545	0.139884	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
363	2	75.022034	-42.128429	10.073915	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
364	2	74.180054	-43.228210	10.290315	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
365	2	75.481102	-41.407768	11.183846	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
366	2	73.798340	-43.591125	11.582500	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
367	2	75.099953	-41.768837	12.476580	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
368	2	74.256905	-42.860668	12.677815	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
369	2	70.377007	-34.785568	1.558481	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
370	2	71.670654	-34.362598	1.889554	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
371	2	69.410721	-34.855991	2.570910	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
372	2	71.993813	-34.024601	3.203910	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
373	2	69.730537	-34.509926	3.883394	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
374	2	71.023636	-34.097260	4.202672	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
375	2	66.606056	-35.772366	-3.807093	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
376	2	65.548492	-36.605030	-4.198068	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
377	2	66.407547	-34.891537	-2.735252	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
378	2	64.324692	-36.564556	-3.530299	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
379	2	65.187004	-34.857868	-2.059670	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
380	2	64.144295	-35.694500	-2.456005	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
381	2	77.937195	-39.239346	4.780356	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
382	2	78.286217	-38.960091	6.108925	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
383	2	77.624054	-38.169979	3.929820	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
384	2	78.308517	-37.646122	6.577985	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
385	2	77.647148	-36.855808	4.397455	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
386	2	77.987160	-36.592327	5.723578	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
387	3	58.156479	-37.444313	-8.942580	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
388	2	59.042656	-36.986397	-10.079196	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
389	2	59.886204	-37.884045	-10.749246	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
390	2	59.018261	-35.648239	-10.493842	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0

391	2	60.689800	-37.453949	-11.808825	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
392	2	59.818848	-35.201534	-11.546641	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
393	2	60.662357	-36.111404	-12.187360	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
394	16	61.516258	-38.257580	-12.542225	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
395	16	59.700909	-33.883823	-11.897748	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
396	3	61.348969	-39.672825	-12.592015	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
397	3	60.344975	-33.371151	-13.059712	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
398	2	62.462669	-40.333870	-11.816863	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
399	2	63.794151	-40.038433	-12.127344	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
400	2	62.203926	-41.273430	-10.813232	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
401	2	64.849831	-40.663136	-11.464224	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
402	2	63.247013	-41.913498	-10.139401	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
403	2	64.571167	-41.607002	-10.470860	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
404	2	59.863445	-34.061253	-14.316494	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
405	2	60.761070	-34.377220	-15.343598	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
406	2	58.518929	-34.412926	-14.478038	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
407	2	60.338795	-35.042187	-16.496466	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
408	2	58.075680	-35.078049	-15.621919	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
409	2	58.991257	-35.392910	-16.631207	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
410	16	66.106789	-40.295094	-11.852272	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
411	16	62.887760	-42.817562	-9.179756	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
412	16	61.304005	-35.313519	-17.426132	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
413	16	56.744205	-35.383045	-15.661792	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
414	3	67.246529	-40.889488	-11.249286	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
415	3	60.986778	-36.035301	-18.609135	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
416	3	63.873718	-43.576180	-8.490973	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
417	3	56.186283	-36.065071	-16.776125	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
418	2	68.461411	-40.255199	-11.879904	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
419	2	68.870766	-38.976513	-11.482786	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
420	2	69.197906	-40.923203	-12.866832	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
421	2	69.996788	-38.382805	-12.049809	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
422	2	70.321434	-40.326164	-13.440292	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
423	2	70.723381	-39.055416	-13.030876	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
424	2	54.711342	-36.229435	-16.496632	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
425	2	54.274704	-37.087997	-15.478518	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
426	2	53.754566	-35.523727	-17.238302	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
427	2	52.914288	-37.236259	-15.206404	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
428	2	52.394257	-35.671349	-16.966562	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
429	2	51.972332	-36.528091	-15.950913	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
430	2	62.269672	-36.189106	-19.391109	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
431	2	62.817570	-35.096611	-20.076683	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
432	2	62.938305	-37.419601	-19.442337	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
433	2	64.006500	-35.230289	-20.794781	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
434	2	64.128403	-37.553780	-20.157940	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
435	2	64.663948	-36.459221	-20.835470	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
436	2	63.149082	-44.440868	-7.487195	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
437	2	62.174347	-45.353470	-7.913151	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
438	2	63.428402	-44.344570	-6.116980	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
439	2	61.488899	-46.145355	-6.991667	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
440	2	62.745659	-45.139553	-5.195346	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
441	2	61.773335	-46.038479	-5.631182	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
442	3	56.919258	-40.875813	-2.145946	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
443	2	58.170025	-41.246952	-2.906767	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
444	2	58.095146	-41.646805	-4.246197	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
445	2	59.428219	-41.181484	-2.296528	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
446	2	59.246243	-41.966724	-4.968151	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
447	2	60.589478	-41.507618	-2.999252	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
448	2	60.491009	-41.905682	-4.335682	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
449	16	61.770096	-41.399696	-2.318409	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
450	16	59.078739	-42.316952	-6.279296	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
451	3	60.142365	-42.121918	-7.205373	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
452	2	60.510387	-40.656372	-7.277609	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
453	2	59.514591	-39.690002	-7.472397	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
454	2	61.841949	-40.233433	-7.154423	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
455	2	59.834518	-38.332157	-7.525724	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
456	2	62.168915	-38.875607	-7.204940	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
457	2	61.159222	-37.929066	-7.371882	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0



458	16	63.449699	-38.417274	-7.107183	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
459	16	58.879562	-37.378330	-7.717875	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
460	3	64.410362	-39.042061	-7.951204	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
461	2	65.577400	-38.095531	-8.108978	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
462	2	65.349991	-36.776886	-8.519526	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
463	2	66.895363	-38.509228	-7.876128	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
464	2	66.404503	-35.881866	-8.699026	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
465	2	67.964920	-37.621372	-8.041814	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
466	2	67.710587	-36.311901	-8.455579	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
467	16	66.071930	-34.623390	-9.117496	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
468	16	69.277184	-37.933323	-7.816782	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
469	3	67.038803	-33.786068	-9.739825	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
470	3	69.667694	-39.257080	-7.476707	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
471	2	67.559853	-34.402725	-11.019145	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
472	2	66.758514	-35.236828	-11.807457	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
473	2	68.869209	-34.140217	-11.441683	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
474	2	67.247025	-35.816845	-12.977632	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
475	2	69.375732	-34.703728	-12.616861	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
476	2	68.556084	-35.539673	-13.380830	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
477	2	71.080482	-39.242035	-6.939989	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
478	2	71.903572	-40.365917	-7.073374	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
479	2	71.579224	-38.134552	-6.244424	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
480	2	73.185234	-40.396408	-6.517963	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
481	2	72.854065	-38.144966	-5.678106	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
482	2	73.655426	-39.282108	-5.815032	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
483	16	66.382278	-36.636578	-13.645798	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
484	16	70.640877	-34.486027	-13.092147	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
485	16	73.901421	-41.544628	-6.715779	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
486	16	73.224167	-37.009216	-5.014652	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
487	3	66.805191	-37.361591	-14.792288	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
488	3	75.077080	-41.835403	-5.968853	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
489	3	71.656288	-33.888592	-12.291133	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
490	3	74.374153	-36.993465	-4.179778	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
491	2	65.633217	-38.199707	-15.247245	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
492	2	64.398987	-37.600655	-15.536694	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
493	2	65.753342	-39.589668	-15.381268	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
494	2	63.309345	-38.372208	-15.940915	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
495	2	64.665535	-40.361317	-15.792229	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
496	2	63.441994	-39.753819	-16.071712	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
497	2	74.469772	-35.602604	-3.598824	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
498	2	73.521751	-35.159847	-2.666981	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
499	2	75.498962	-34.730202	-3.977888	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
500	2	73.599312	-33.876480	-2.125577	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
501	2	75.578575	-33.446682	-3.435787	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
502	2	74.629066	-33.018402	-2.508806	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
503	2	74.719574	-42.195572	-4.545196	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
504	2	73.764862	-43.189297	-4.287058	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
505	2	75.352081	-41.574802	-3.459209	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
506	2	73.448189	-43.553024	-2.977907	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
507	2	75.037247	-41.940441	-2.149556	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
508	2	74.086639	-42.930588	-1.906819	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
509	2	72.136803	-34.868763	-11.245698	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
510	2	71.976051	-34.623001	-9.874979	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
511	2	72.775391	-36.051609	-11.643610	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
512	2	72.425522	-35.544525	-8.928082	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
513	2	73.225700	-36.973415	-10.698040	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
514	2	73.048767	-36.721970	-9.338675	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
515	3	41.988297	-34.024635	12.803845	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
516	2	40.601776	-34.618420	12.897466	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
517	2	40.069786	-34.934601	14.154042	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
518	2	39.808338	-34.839138	11.765036	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
519	2	38.786579	-35.468403	14.288472	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
520	2	38.519127	-35.360790	11.879670	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
521	2	38.014763	-35.680721	13.143098	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
522	16	38.385868	-35.764942	15.562042	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
523	16	37.820305	-35.560139	10.722503	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
524	3	37.178978	-36.470345	15.829932	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0

525	3	36.437717	-35.226562	10.672914	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
526	2	36.005375	-35.524666	15.903059	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
527	2	36.011539	-34.484787	16.835430	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
528	2	34.880436	-35.681099	15.087134	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
529	2	34.920815	-33.627602	16.975409	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
530	2	33.782051	-34.827000	15.197746	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
531	2	33.804398	-33.805096	16.152544	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
532	2	36.286316	-33.722240	10.675649	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
533	2	36.069550	-33.020233	11.868293	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
534	2	36.343086	-33.008434	9.470846	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
535	2	35.916626	-31.630112	11.864498	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
536	2	36.192108	-31.618397	9.451260	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
537	2	35.984806	-30.941643	10.653320	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
538	16	35.052277	-32.633183	17.903904	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
539	16	32.749252	-35.057735	14.331078	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
540	16	35.686981	-30.877131	12.982072	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
541	16	36.224388	-30.852438	8.319143	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
542	3	33.926250	-32.028477	18.527721	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
543	3	35.387550	-31.528509	14.208390	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
544	3	31.643084	-34.168449	14.237041	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
545	3	36.306587	-31.473618	7.043721	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
546	2	33.415249	-32.941452	19.616810	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
547	2	34.068913	-32.991692	20.855423	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
548	2	32.284111	-33.743526	19.421175	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
549	2	33.601360	-33.820728	21.875349	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
550	2	31.815733	-34.574509	20.439205	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
551	2	32.472252	-34.612358	21.668768	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
552	2	36.232750	-30.382004	6.002872	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
553	2	35.003105	-29.790499	5.684030	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
554	2	37.382633	-29.948347	5.329521	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
555	2	34.922390	-28.794863	4.710080	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
556	2	37.303684	-28.949514	4.357956	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
557	2	36.073021	-28.373283	4.045226	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
558	2	34.973190	-30.465952	15.197795	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
559	2	35.906815	-29.888166	16.068048	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
560	2	33.636833	-30.049433	15.269505	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
561	2	35.513359	-28.917019	16.989557	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
562	2	33.242596	-29.078978	16.191034	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
563	2	34.180714	-28.511734	17.052494	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
564	2	30.717049	-34.306320	15.422996	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
565	2	30.091593	-33.177395	15.970237	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
566	2	30.448263	-35.561020	15.986093	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
567	2	29.226671	-33.299976	17.058363	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
568	2	29.585621	-35.685177	17.075176	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
569	2	28.973412	-34.553963	17.612963	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
570	3	47.246014	-35.726910	11.339565	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
571	2	45.766994	-36.035465	11.359544	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
572	2	44.822239	-35.004780	11.415964	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
573	2	45.305862	-37.355328	11.337525	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
574	2	43.457142	-35.290340	11.459052	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
575	2	43.943645	-37.658241	11.349915	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
576	2	43.016266	-36.614437	11.417572	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
577	16	43.627472	-38.987583	11.289462	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
578	16	42.577606	-34.251839	11.525493	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
579	3	42.282738	-39.429985	11.160834	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
580	2	41.506275	-39.272018	12.447517	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
581	2	40.105412	-39.207867	12.404615	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
582	2	42.147724	-39.202671	13.692935	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
583	2	39.365971	-39.055344	13.577754	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
584	2	41.416813	-39.029106	14.867874	1 " " X " "	2	0.00015	0.00015	" " " C " " "	6	0	0	1	C	0
585	2	40.027908	-38.951038	14.799846	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0
586	16	38.007107	-38.992065	13.640051	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
587	16	42.087170	-38.980297	16.055798	1 " " X " "	70	-0.17255	-0.17255	" " " O " " "	8	0	0	1	O	0
588	3	37.151836	-39.439957	12.598400	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
589	3	42.030087	-37.760525	16.788874	1 " " X " "	2	0.29741	0.29741	" " " C " " "	6	0	0	1	C	0
590	2	35.738693	-39.282448	13.116893	1 " " X " "	2	-0.12501	-0.12501	" " " C " " "	6	0	0	1	C	0
591	2	34.680656	-38.951710	12.261705	1 " " X " "	2	-0.11346	-0.11346	" " " C " " "	6	0	0	1	C	0

592	2	35.464626	-39.428402	14.483467	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
593	2	33.387127	-38.751122	12.753301	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
594	2	34.189835	-39.198147	14.997581	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
595	2	33.149723	-38.864830	14.126871	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
596	2	40.826157	-37.654427	17.698612	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
597	2	40.401138	-36.390011	18.127066	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
598	2	40.118740	-38.776123	18.147463	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
599	2	39.300217	-36.236240	18.971943	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
600	2	38.987999	-38.642418	18.955454	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
601	2	38.585762	-37.369389	19.373072	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
602	16	32.428192	-38.431309	11.831952	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
603	16	34.061661	-39.282856	16.354834	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
604	16	38.994534	-34.957039	19.350203	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
605	16	38.329731	-39.796207	19.278587	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
606	3	31.108755	-38.062405	12.217221	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
607	3	37.950760	-34.711365	20.284933	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
608	3	32.985161	-38.611706	16.997942	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
609	3	36.984344	-39.725349	19.733953	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
610	2	30.326178	-39.249981	12.728993	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
611	2	30.418306	-40.501255	12.104373	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
612	2	29.476671	-39.113819	13.836286	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
613	2	29.690958	-41.591846	12.582331	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
614	2	28.749643	-40.203850	14.315392	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
615	2	28.857038	-41.445011	13.689830	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
616	2	36.440235	-41.133495	19.752634	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
617	2	35.995541	-41.734138	18.567301	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
618	2	36.355659	-41.858131	20.948757	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
619	2	35.476952	-43.029156	18.576839	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
620	2	35.837818	-43.153866	20.959141	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
621	2	35.397518	-43.740707	19.773308	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
622	2	37.917988	-33.233829	20.601534	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
623	2	37.934570	-32.271751	19.582150	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
624	2	37.851448	-32.796425	21.932142	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
625	2	37.883308	-30.910473	19.882839	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
626	2	37.802032	-31.435055	22.234484	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
627	2	37.816658	-30.489895	21.209953	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
628	2	33.342499	-38.512653	18.461182	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
629	2	33.949097	-37.354961	18.967224	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
630	2	33.084587	-39.575680	19.336306	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
631	2	34.289238	-37.262245	20.316771	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
632	2	33.422497	-39.482368	20.687099	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
633	2	34.024326	-38.324818	21.179384	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
634	3	52.142254	-39.632053	11.236857	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
635	2	53.401688	-39.189869	11.944022	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
636	2	54.006741	-40.009045	12.905062	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
637	2	53.973156	-37.939877	11.672516	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
638	2	55.155880	-39.589878	13.577538	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
639	2	55.120178	-37.508385	12.341372	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
640	2	55.722557	-38.350349	13.278561	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
641	16	55.724796	-40.374954	14.537312	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
642	16	55.579662	-36.256237	12.046178	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
643	3	54.987164	-40.499859	15.754001	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
644	3	56.017155	-35.421894	13.117902	1	"	"	X	"	2	0.29741	0.29741	"	"	C	"	"	6	0	0	1	C	0
645	2	55.348782	-39.362110	16.682377	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
646	2	56.104603	-39.583015	17.840260	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
647	2	54.935242	-38.055477	16.401863	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
648	2	56.451290	-38.531532	18.692081	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
649	2	55.299160	-36.986893	17.219910	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
650	2	56.052742	-37.229507	18.371893	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
651	2	57.517765	-35.503826	13.268089	1	"	"	X	"	2	-0.12501	-0.12501	"	"	C	"	"	6	0	0	1	C	0
652	2	58.106007	-35.930122	14.464982	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
653	2	58.349613	-35.126038	12.207723	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
654	2	59.495872	-35.997593	14.596095	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
655	2	59.739559	-35.177975	12.323630	1	"	"	X	"	2	0.00015	0.00015	"	"	C	"	"	6	0	0	1	C	0
656	2	60.305344	-35.618950	13.522728	1	"	"	X	"	2	-0.11346	-0.11346	"	"	C	"	"	6	0	0	1	C	0
657	16	57.171577	-38.862320	19.806355	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0
658	16	54.897141	-35.750031	16.802563	1	"	"	X	"	70	-0.17255	-0.17255	"	"	O	"	"	8	0	0	1	O	0



659	16	60.137268	-36.419750	15.726452	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
660	16	60.458088	-34.780289	11.230944	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
661	3	57.694630	-37.845501	20.651119	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
662	3	59.393040	-36.908630	16.834244	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
663	3	55.363876	-34.587101	17.470881	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
664	3	61.879173	-34.829014	11.241917	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
665	2	58.331985	-38.516697	21.844007	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
666	2	59.386898	-39.421322	21.669403	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
667	2	57.887886	-38.245132	23.145424	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
668	2	59.984547	-40.041039	22.766993	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
669	2	58.483307	-38.865498	24.244211	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
670	2	59.532684	-39.764153	24.056540	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
671	2	62.347980	-34.298557	9.907823	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
672	2	62.139618	-35.042252	8.738578	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
673	2	62.995220	-33.059170	9.810719	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
674	2	62.566734	-34.558720	7.501585	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
675	2	63.422359	-32.574764	8.573734	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
676	2	63.208908	-33.324127	7.417663	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
677	2	60.398621	-37.372375	17.859798	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
678	2	60.880943	-38.687637	17.842136	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
679	2	60.873779	-36.492878	18.841356	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
680	2	61.819279	-39.113537	18.782650	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
681	2	61.807396	-36.919552	19.786198	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
682	2	62.282509	-38.230072	19.756863	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
683	2	55.046410	-33.410511	16.580158	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
684	2	56.035355	-32.843796	15.764704	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
685	2	53.755375	-32.869194	16.548204	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
686	2	55.738991	-31.761595	14.935814	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
687	2	53.457802	-31.786459	15.720463	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
688	2	54.449638	-31.231466	14.912787	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
689	3	47.960098	-35.674614	5.183897	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
690	2	47.956722	-36.303268	6.557302	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
691	2	48.103344	-37.688725	6.695127	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
692	2	47.789494	-35.529499	7.712153	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
693	2	48.075523	-38.297470	7.950420	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
694	2	47.761349	-36.117729	8.979177	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
695	2	47.907253	-37.504208	9.088548	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
696	16	47.618038	-35.267971	10.043302	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
697	16	48.247677	-39.654560	7.977825	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
698	3	47.508560	-40.463242	8.887735	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
699	2	48.041527	-40.401321	10.300203	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
700	2	49.400249	-40.198994	10.573730	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
701	2	47.151939	-40.527573	11.374433	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
702	2	49.854843	-40.086876	11.891059	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
703	2	47.587372	-40.419601	12.695461	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
704	2	48.944069	-40.200108	12.943468	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
705	16	46.625053	-40.524494	13.661725	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
706	16	51.153782	-39.841724	12.237530	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
707	3	46.927975	-40.345367	15.039681	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
708	2	47.282265	-38.907585	15.345034	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
709	2	48.410049	-38.601151	16.116783	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
710	2	46.476013	-37.854492	14.894993	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
711	2	48.743690	-37.280148	16.419130	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
712	2	46.788841	-36.525875	15.191755	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
713	2	47.934448	-36.245129	15.942430	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
714	16	49.854317	-37.091129	17.194824	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
715	16	45.924511	-35.571175	14.728405	1 " " X " "	70	-0.17255	-0.17255	" " O " "	"	8	0	0	1	0	0
716	3	50.181850	-35.793163	17.675842	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
717	3	46.015556	-34.218456	15.163193	1 " " X " "	2	0.29741	0.29741	" " C " "	"	6	0	0	1	0	0
718	2	51.281822	-35.877121	18.709978	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
719	2	51.718464	-34.699993	19.330418	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
720	2	51.862652	-37.088230	19.105238	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
721	2	52.700874	-34.718853	20.322086	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
722	2	52.840565	-37.131145	20.100605	1 " " X " "	2	0.00015	0.00015	" " C " "	"	6	0	0	1	0	0
723	2	53.261696	-35.941086	20.701542	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0
724	2	45.770977	-34.111153	16.652220	1 " " X " "	2	-0.12501	-0.12501	" " C " "	"	6	0	0	1	0	0
725	2	46.602348	-33.335068	17.469969	1 " " X " "	2	-0.11346	-0.11346	" " C " "	"	6	0	0	1	0	0

726	2	44.704262	-34.794498	17.246908	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
727	2	46.391365	-33.253548	18.848625	1 " " X " "	2	0.00015	0.00015	" " C " " "	6	0	0	1	C	0
728	2	44.480297	-34.732754	18.623320	1 " " X " "	2	0.00015	0.00015	" " C " " "	6	0	0	1	C	0
729	2	45.329124	-33.959988	19.419901	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
730	16	53.027523	-33.509571	20.871845	1 " " X " "	70	-0.17255	-0.17255	" " O " " "	8	0	0	1	O	0
731	16	53.316574	-38.370499	20.429646	1 " " X " "	70	-0.17255	-0.17255	" " O " " "	8	0	0	1	O	0
732	16	47.260399	-32.466877	19.554367	1 " " X " "	70	-0.17255	-0.17255	" " O " " "	8	0	0	1	O	0
733	16	43.422874	-35.455544	19.101748	1 " " X " "	70	-0.17255	-0.17255	" " O " " "	8	0	0	1	O	0
734	3	53.978264	-33.388138	21.924435	1 " " X " "	2	0.29741	0.29741	" " C " " "	6	0	0	1	C	0
735	3	47.115219	-32.262222	20.955942	1 " " X " "	2	0.29741	0.29741	" " C " " "	6	0	0	1	C	0
736	3	53.992157	-38.588928	21.661894	1 " " X " "	2	0.29741	0.29741	" " C " " "	6	0	0	1	C	0
737	3	43.218464	-35.649090	20.496250	1 " " X " "	2	0.29741	0.29741	" " C " " "	6	0	0	1	C	0
738	2	55.387737	-33.471947	21.385017	1 " " X " "	2	-0.12501	-0.12501	" " C " " "	6	0	0	1	C	0
739	2	55.785912	-32.661602	20.312649	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
740	2	56.333778	-34.328030	21.965574	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
741	2	57.090405	-32.718094	19.820818	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
742	2	57.640148	-34.381847	21.477221	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
743	2	58.018635	-33.581032	20.400894	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
744	2	42.700760	-34.407967	21.186672	1 " " X " "	2	-0.12501	-0.12501	" " C " " "	6	0	0	1	C	0
745	2	42.966648	-34.212105	22.549318	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
746	2	41.940018	-33.445683	20.508762	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
747	2	42.495678	-33.079494	23.213934	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
748	2	41.468182	-32.313019	21.172443	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
749	2	41.745632	-32.127514	22.525572	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
750	2	47.501347	-33.497715	21.736759	1 " " X " "	2	-0.12501	-0.12501	" " C " " "	6	0	0	1	C	0
751	2	48.659409	-34.218502	21.416840	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
752	2	46.717785	-33.933418	22.814173	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
753	2	49.020111	-35.353413	22.144022	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
754	2	47.074677	-35.069317	23.541624	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
755	2	48.225708	-35.781361	23.206717	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
756	2	53.069935	-38.328968	22.830904	1 " " X " "	2	-0.12501	-0.12501	" " C " " "	6	0	0	1	C	0
757	2	53.475018	-37.518494	23.900560	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
758	2	51.791233	-38.901787	22.869400	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
759	2	52.618607	-37.277306	24.975313	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
760	2	50.935131	-38.663132	23.944759	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
761	2	51.347057	-37.848480	24.998362	1 " " X " "	2	-0.11346	-0.11346	" " C " " "	6	0	0	1	C	0
762	41	51.089611	-37.073406	3.186746	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
763	41	47.609612	-34.555122	2.902018	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
764	41	51.342651	-36.043667	-2.538299	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
765	41	55.617519	-37.354572	-3.499959	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
766	41	53.652843	-36.109673	-2.656197	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
767	41	54.879032	-40.484577	-0.596487	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
768	41	52.922512	-39.251358	0.237770	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
769	41	50.729008	-33.405022	-6.347218	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
770	41	49.840767	-31.865187	-6.298044	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
771	41	48.104733	-31.369081	-8.117526	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
772	41	50.688934	-34.837204	-8.323970	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
773	41	48.470253	-33.571560	-11.794432	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
774	41	47.846699	-31.410744	-12.561188	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
775	41	46.513866	-32.553009	-12.152923	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
776	41	50.325520	-36.765892	-12.303733	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
777	41	48.720978	-36.064793	-12.005835	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
778	41	47.301723	-28.853107	-11.715566	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
779	41	44.360645	-31.836395	-12.781922	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
780	41	43.359703	-27.647371	-12.999034	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
781	41	48.056797	-34.851303	-13.930346	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
782	41	52.166355	-34.583942	-12.648710	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
783	41	50.765427	-32.193039	-15.979210	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0
784	41	44.748844	-25.862961	-13.676243	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
785	41	45.745975	-24.820639	-12.640123	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
786	41	47.416016	-33.257874	-17.726725	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
787	41	49.127224	-33.743790	-17.650284	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
788	41	41.913540	-28.573257	-14.528664	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
789	41	41.155708	-28.691547	-12.896603	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
790	41	53.821354	-33.088329	-12.751514	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
791	41	54.164520	-34.269226	-14.068609	1 " " X " "	21	0.00000	0.00000	" " H " " "	1	0	0	1	H	0
792	41	42.636383	-24.686707	-13.319289	1 " " X " "	21	0.11346	0.11346	" " H " " "	1	0	0	1	H	0

793	41	44.922306	-26.019714	-9.882913	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
794	41	40.728565	-24.141035	-11.831553	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
795	41	43.002289	-25.478544	-8.403734	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
796	41	40.894821	-24.542238	-9.368544	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
797	41	54.928150	-32.840355	-16.391172	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
798	41	55.694233	-31.728134	-12.272427	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
799	41	56.908630	-31.517632	-17.111170	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
800	41	57.667828	-30.406698	-13.001164	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
801	41	58.285442	-30.297285	-15.419960	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
802	41	49.300617	-36.098900	-18.064884	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
803	41	45.994949	-34.653297	-15.662522	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
804	41	48.541367	-38.434792	-17.695368	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
805	41	45.244816	-36.993744	-15.294712	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
806	41	46.513943	-38.894295	-16.307978	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
807	41	40.266979	-28.910873	-16.208151	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
808	41	40.170254	-31.392988	-12.656730	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
809	41	38.363327	-30.197609	-17.152006	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
810	41	38.262886	-32.670948	-13.605979	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
811	41	37.351330	-32.079868	-15.857653	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
812	41	44.690525	-29.702517	-4.213677	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
813	41	46.337532	-29.136921	-4.562038	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
814	41	48.057613	-31.495571	-4.341429	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
815	41	44.096313	-31.152292	-6.049037	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
816	41	46.760170	-34.321102	-7.313862	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
817	41	45.502659	-33.967632	-9.153286	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
818	41	44.663841	-35.151783	-8.085153	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
819	41	44.696476	-34.119591	-11.329078	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
820	41	41.876270	-34.435604	-8.068213	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
821	41	40.469196	-34.513985	-12.145322	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
822	41	41.321262	-33.342438	-14.077032	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
823	41	41.371761	-35.136955	-14.206398	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
824	41	38.191032	-34.049057	-8.442710	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
825	41	39.805206	-33.616924	-7.848741	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
826	41	42.399738	-36.149643	-16.146122	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
827	41	43.189522	-31.993654	-15.251672	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
828	41	44.605999	-33.718063	-18.942909	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
829	41	40.996632	-31.667065	-8.833782	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
830	41	37.074436	-32.755520	-10.247485	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
831	41	38.721981	-28.869545	-11.196914	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
832	41	45.619678	-35.968594	-18.917065	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
833	41	44.804501	-37.418457	-19.536310	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
834	41	42.709579	-28.431114	-9.233582	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
835	41	42.546379	-30.186993	-9.077333	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
836	41	45.372662	-31.735291	-19.270247	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
837	41	45.173622	-30.061338	-18.721996	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
838	41	36.420181	-28.499599	-11.612206	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
839	41	37.270844	-29.285498	-12.992173	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
840	41	42.240543	-36.229706	-20.661989	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
841	41	46.371403	-34.948254	-20.971224	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
842	41	41.745251	-35.137817	-22.839916	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
843	41	45.865990	-33.862801	-23.149544	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
844	41	43.553463	-33.952183	-24.092230	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
845	41	35.996113	-29.302521	-14.982798	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
846	41	33.936451	-29.739073	-11.195293	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
847	41	33.824829	-29.480886	-16.179689	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
848	41	31.769180	-29.924212	-12.400941	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
849	41	31.703020	-29.792498	-14.894592	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
850	41	41.882980	-30.982702	-6.842761	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
851	41	40.806587	-26.966709	-8.063043	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
852	41	40.902000	-30.559542	-4.603274	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
853	41	39.833111	-26.549919	-5.813085	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
854	41	39.871452	-28.347679	-4.076600	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
855	41	43.883228	-32.209110	-21.114170	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
856	41	42.501297	-29.589300	-17.950764	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
857	41	41.692764	-31.974293	-22.261766	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
858	41	40.311275	-29.356590	-19.107857	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
859	41	39.897320	-30.548744	-21.264954	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0

860	41	37.662441	-37.768200	0.073904	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
861	41	37.270321	-37.659096	-1.652638	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
862	41	35.080963	-36.619217	-1.848616	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
863	41	37.849510	-35.108654	1.112106	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
864	41	34.038612	-33.176796	0.535078	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
865	41	32.436352	-33.005524	-1.138139	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
866	41	31.957842	-34.232746	0.096634	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
867	41	36.483006	-31.260225	2.643815	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
868	41	35.684544	-31.411711	1.067898	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
869	41	31.394512	-36.532463	-2.002676	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
870	41	30.160942	-32.398571	-1.718406	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
871	41	27.653214	-35.263950	-3.732367	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
872	41	33.440262	-30.672520	1.411502	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
873	41	35.221012	-33.250439	4.387771	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
874	41	31.094662	-32.030319	4.755549	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
875	41	27.298201	-37.580658	-3.412754	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
876	41	28.264690	-38.889114	-4.126585	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
877	41	29.222937	-29.783630	2.493367	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
878	41	29.852160	-30.252195	4.083547	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
879	41	26.097103	-33.615471	-3.191955	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
880	41	26.964790	-33.234367	-4.726511	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
881	41	31.778421	-32.237480	6.931624	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
882	41	31.132465	-33.796543	6.302821	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
883	41	30.229710	-37.372459	-5.848746	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
884	41	25.962862	-36.841736	-5.281695	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
885	41	30.048294	-36.353207	-8.109506	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
886	41	25.794416	-35.823708	-7.541396	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
887	41	27.832016	-35.575508	-8.963789	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
888	41	32.369526	-35.985794	7.230444	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
889	41	32.462475	-32.121284	9.193679	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
890	41	32.919144	-37.088383	9.391923	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
891	41	33.000751	-33.231438	11.347205	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
892	41	33.227127	-35.715416	11.460499	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
893	41	29.838770	-32.144989	0.776105	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
894	41	28.295729	-31.957247	4.821068	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
895	41	28.722116	-34.347042	0.457530	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
896	41	27.186979	-34.157356	4.495274	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
897	41	27.395540	-35.360344	2.314988	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
898	41	25.373638	-31.638357	-1.681615	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
899	41	26.576649	-31.109938	-5.813112	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
900	41	24.277056	-29.406120	-1.719720	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
901	41	25.478676	-28.880625	-5.842117	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
902	41	24.328424	-28.018124	-3.798109	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
903	41	47.055828	-32.646488	1.459032	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
904	41	46.075287	-34.158150	1.413493	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
905	41	44.318340	-34.405457	-0.158278	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
906	41	47.312504	-31.353052	-0.821947	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
907	41	43.823174	-31.552404	-3.353720	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
908	41	42.353603	-33.178032	-4.031132	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
909	41	41.586662	-32.138744	-2.766024	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
910	41	40.906975	-34.961132	-1.120606	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
911	41	40.034817	-33.298290	-5.024728	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
912	41	37.369350	-36.188892	-3.260835	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
913	41	35.947895	-34.533562	-6.181942	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
914	41	35.988586	-35.069557	-4.493209	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
915	41	35.489712	-33.390079	-2.815418	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
916	41	36.937794	-32.155651	-6.686196	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
917	41	35.617859	-29.190966	-3.849046	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
918	41	34.279781	-29.722532	-0.514632	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
919	41	34.779926	-28.942507	-2.011031	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
920	41	37.936527	-29.867331	-7.646946	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
921	41	36.321346	-30.588717	-7.979695	1 " " X " "	21	0.00000	0.00000	" " " H " " "	1	0	0	1	H	0
922	41	31.995604	-29.397190	-0.130672	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
923	41	33.265598	-30.335878	-4.163206	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
924	41	29.082037	-29.908192	-3.269850	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
925	41	34.318520	-29.124538	-8.403848	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0
926	41	38.354256	-27.578121	-8.429971	1 " " X " "	21	0.11346	0.11346	" " " H " " "	1	0	0	1	H	0

927	41	35.186821	-25.386759	-10.371573	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
928	41	27.841589	-28.725060	-1.737858	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
929	41	27.876652	-30.480894	-1.331588	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
930	41	32.919064	-25.209969	-10.209883	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
931	41	33.325912	-26.272930	-11.608038	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
932	41	29.118755	-31.412661	-5.146601	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
933	41	29.054520	-29.658384	-5.558578	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
934	41	36.733105	-23.848896	-10.502505	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
935	41	38.476597	-23.799709	-10.809587	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
936	41	26.744766	-31.249681	0.633870	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
937	41	27.744473	-27.047037	0.273747	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
938	41	25.476904	-30.767561	2.713770	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
939	41	26.468962	-26.571987	2.357985	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
940	41	25.332994	-28.428961	3.585828	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
941	41	35.584389	-24.119373	-12.619196	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
942	41	39.265526	-26.312841	-11.953066	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
943	41	35.340321	-25.214619	-14.835786	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
944	41	39.020157	-27.384680	-14.181103	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
945	41	37.058640	-26.846384	-15.628425	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
946	41	30.775589	-26.017578	-8.788857	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
947	41	31.503742	-27.025520	-12.941451	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
948	41	28.348339	-26.464506	-9.111627	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
949	41	29.078878	-27.473021	-13.253908	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
950	41	27.492342	-27.195507	-11.342711	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
951	41	30.334412	-28.900627	-7.719438	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
952	41	29.237671	-33.021339	-6.925518	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
953	41	30.552839	-29.429293	-10.138182	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
954	41	29.461069	-33.538368	-9.347578	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
955	41	30.117296	-31.748514	-10.962046	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
956	41	67.108986	-36.812805	-0.425554	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
957	41	67.822632	-38.425129	-0.661649	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
958	41	69.108650	-38.545227	1.399434	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
959	41	64.906456	-37.529675	1.600783	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
960	41	67.105064	-38.407021	5.214370	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
961	41	69.352722	-37.121086	5.195850	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
962	41	69.351448	-38.728077	6.009436	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
963	41	63.378128	-38.380955	5.572875	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
964	41	64.907890	-39.277863	5.526990	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
965	41	71.542946	-37.811989	3.121852	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
966	41	71.313911	-38.269047	7.401282	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
967	41	75.158508	-37.788033	5.482453	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
968	41	65.913658	-35.843842	5.313774	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
969	41	64.132835	-38.669132	8.052817	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
970	41	66.123665	-35.162495	9.573365	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
971	41	72.997246	-36.938694	1.579236	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
972	41	73.191376	-38.725849	1.647621	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
973	41	67.601929	-32.413063	7.597298	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
974	41	66.461624	-33.074089	8.783317	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
975	41	72.930473	-39.256905	9.049156	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
976	41	72.568817	-37.491177	9.122641	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
977	41	63.124187	-38.407368	10.080638	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
978	41	64.665825	-39.312916	10.325521	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
979	41	75.339249	-39.796314	0.901962	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
980	41	74.686249	-35.532799	0.486041	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
981	41	77.247414	-39.653412	-0.690176	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
982	41	76.589310	-35.400414	-1.105167	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
983	41	77.875748	-37.457790	-1.701949	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
984	41	65.964149	-38.040440	12.598949	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
985	41	61.732475	-38.749710	11.965433	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
986	41	65.584579	-38.020321	15.057570	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
987	41	61.368214	-38.736919	14.420959	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
988	41	63.286621	-38.364521	15.977568	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
989	41	67.764664	-33.428814	10.800150	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
990	41	69.465782	-34.588799	6.987267	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
991	41	69.739388	-34.388088	11.965096	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
992	41	71.442230	-35.528374	8.155445	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
993	41	71.586624	-35.440952	10.652615	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0

994	41	72.865700	-38.368336	11.657214	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
995	41	76.120857	-37.711014	8.864420	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
996	41	74.445526	-38.070930	13.553580	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
997	41	77.684296	-37.418350	10.763184	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
998	41	76.859322	-37.594406	13.115723	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
999	41	63.059299	-42.694756	-3.321743	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1000	41	63.084999	-40.985378	-3.889275	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1001	41	63.886806	-39.172405	-2.264070	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1002	41	64.593544	-43.383289	-1.577148	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1003	41	67.009430	-40.425285	0.430924	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1004	41	67.573235	-43.867386	1.655128	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1005	41	66.952438	-42.228699	1.936852	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1006	41	69.411171	-42.159996	2.810034	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1007	41	68.452522	-42.427563	-1.396451	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1008	41	72.326523	-40.992512	-0.142470	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1009	41	71.525093	-42.761963	3.719102	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1010	41	71.015717	-41.100334	4.204932	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1011	41	72.514153	-40.486389	-2.166391	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1012	41	71.770584	-40.629845	-3.763235	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1013	41	72.212029	-41.795181	6.369947	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1014	41	74.348946	-41.244049	2.647787	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1015	41	76.478203	-41.162350	6.392616	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1016	41	69.731186	-39.333008	-4.372099	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1017	41	71.773750	-38.643970	-0.630006	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1018	41	69.075020	-35.670010	-2.196209	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1019	41	76.103569	-42.531651	8.263571	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1020	41	75.987869	-40.777748	8.670103	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1021	41	68.621033	-35.021408	-4.255332	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1022	41	67.700974	-35.625042	-5.639635	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1023	41	78.691368	-40.746437	3.458867	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1024	41	78.189949	-41.404724	5.025311	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1025	41	70.359634	-34.375629	-0.567148	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1026	41	68.934334	-35.295967	0.036170	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1027	41	73.811241	-43.816383	9.432148	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1028	41	76.151123	-40.543026	11.041957	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1029	41	73.132706	-44.457790	11.738041	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1030	41	75.466614	-41.187923	13.340523	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1031	41	73.955399	-43.146732	13.700287	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1032	41	72.446548	-34.302040	1.107680	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1033	41	68.385223	-35.190781	2.337854	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1034	41	73.018837	-33.700985	3.453787	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1035	41	68.957397	-34.568504	4.668020	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1036	41	71.280350	-33.830399	5.241974	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1037	41	65.679291	-37.297760	-5.047412	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1038	41	67.215858	-34.211655	-2.417222	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1039	41	63.499294	-37.221863	-3.853887	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1040	41	65.044334	-34.163773	-1.213523	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1041	41	63.177856	-35.665188	-1.924215	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1042	41	78.548851	-39.781075	6.797721	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1043	41	77.350777	-38.364132	2.878202	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1044	41	78.582329	-37.440392	7.627045	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1045	41	77.391167	-36.025684	3.716713	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1046	41	78.002441	-35.553474	6.095305	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1047	41	57.267448	-36.783268	-8.862344	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1048	41	57.762791	-38.465790	-9.124465	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1049	41	59.912209	-38.935848	-10.422961	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1050	41	58.352112	-34.929634	-9.986721	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1051	41	61.309727	-35.793678	-13.018648	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1052	41	61.417717	-39.993114	-13.653697	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1053	41	60.342091	-39.983299	-12.248810	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1054	41	60.116840	-32.286484	-13.136503	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1055	41	61.446423	-33.450047	-12.940904	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1056	41	64.018875	-39.301586	-12.917181	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1057	41	61.162048	-41.524712	-10.552426	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1058	41	65.397118	-42.107738	-9.946390	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1059	41	61.826561	-34.109074	-15.241771	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1060	41	57.790665	-34.169338	-13.686025	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0



1061	41	58.649506	-35.918449	-17.534170	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1062	41	67.248718	-40.703876	-10.153685	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1063	41	67.244934	-41.987476	-11.418037	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1064	41	60.237713	-35.480316	-19.213863	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1065	41	60.562557	-37.029461	-18.352642	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1066	41	64.588402	-42.899151	-7.976345	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1067	41	64.439369	-44.214897	-9.202994	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1068	41	56.348495	-35.479767	-17.706160	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1069	41	56.661785	-37.061794	-16.899794	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1070	41	68.298630	-38.426540	-10.716483	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1071	41	68.891052	-41.929417	-13.200188	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1072	41	70.307175	-37.376884	-11.720586	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1073	41	70.893738	-40.860855	-14.217941	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1074	41	71.612434	-38.582802	-13.481863	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1075	41	55.011864	-37.650036	-14.879436	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1076	41	54.071793	-34.838352	-18.042818	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1077	41	52.582756	-37.911434	-14.398989	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1078	41	51.651283	-35.103958	-17.552223	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1079	41	50.896423	-36.639359	-15.732074	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1080	41	62.308403	-34.117512	-20.048157	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1081	41	62.528809	-38.295280	-18.910154	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1082	41	64.428291	-34.361603	-21.329597	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1083	41	64.647079	-38.527775	-20.186165	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1084	41	65.605560	-36.565075	-21.401533	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1085	41	61.938953	-45.446152	-8.987592	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1086	41	64.193291	-43.636036	-5.755399	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1087	41	60.720657	-46.857269	-7.339877	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1088	41	62.974316	-45.058624	-4.118825	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1089	41	61.232136	-46.665245	-4.901588	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1090	41	56.131439	-41.642368	-2.309469	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1091	41	57.128994	-40.814964	-1.056828	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1092	41	57.113800	-41.693577	-4.748678	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1093	41	59.511879	-40.860744	-1.244220	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1094	41	61.397209	-42.172470	-4.896661	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1095	41	59.804386	-42.462219	-8.207504	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1096	41	61.005989	-42.761673	-6.937842	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1097	41	58.463314	-40.007885	-7.569676	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1098	41	62.637234	-40.980911	-7.004752	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1099	41	61.413757	-36.857037	-7.413741	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1100	41	64.730270	-40.010624	-7.512783	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1101	41	63.971043	-39.240906	-8.952073	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1102	41	64.319107	-36.437309	-8.718455	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1103	41	67.072868	-39.548443	-7.559405	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1104	41	68.563095	-35.626663	-8.584971	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1105	41	66.555267	-32.815578	-9.982404	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1106	41	67.857109	-33.555595	-9.025846	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1107	41	69.009239	-39.666687	-6.681930	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1108	41	69.585411	-39.910431	-8.371500	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1109	41	65.722107	-35.456142	-11.500031	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1110	41	69.493095	-33.472229	-10.829649	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1111	41	68.967430	-35.981827	-14.301896	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1112	41	71.532082	-41.253960	-7.612484	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1113	41	70.950706	-37.237366	-6.115362	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1114	41	74.661736	-39.295387	-5.374731	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1115	41	67.104218	-36.664001	-15.603930	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1116	41	67.675636	-38.003521	-14.538249	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1117	41	75.579041	-42.708504	-6.438611	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1118	41	75.802284	-40.998795	-6.033483	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1119	41	72.509529	-33.624012	-12.952253	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1120	41	71.306152	-32.930817	-11.855370	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1121	41	74.273308	-37.745262	-3.367157	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1122	41	75.284691	-37.232933	-4.768392	1	"	X	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1123	41	64.279633	-36.507858	-15.438059	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1124	41	66.712746	-40.086346	-15.155378	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1125	41	62.341648	-37.887302	-16.155502	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1126	41	64.772469	-41.455307	-15.890698	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1127	41	62.580940	-40.364616	-16.392460	1	"	X	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0

1128	41	72.704651	-35.832458	-2.356340	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1129	41	76.257408	-35.054256	-4.711090	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1130	41	72.845901	-33.540607	-1.393022	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1131	41	76.394524	-32.769138	-3.741319	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1132	41	74.692162	-32.003529	-2.080088	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1133	41	73.257278	-43.695965	-5.125972	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1134	41	76.112907	-40.794312	-3.631803	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1135	41	72.693398	-44.335880	-2.789538	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1136	41	75.543274	-41.448143	-1.302390	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1137	41	73.839264	-43.219727	-0.870939	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1138	41	71.489754	-33.694870	-9.530305	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1139	41	72.919304	-36.263790	-12.717023	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1140	41	72.287567	-35.342350	-7.851827	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1141	41	73.718620	-37.904682	-11.026362	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1142	41	73.401611	-37.452236	-8.590525	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1143	41	41.912106	-32.926964	12.960515	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1144	41	42.647766	-34.413536	13.609827	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1145	41	40.674259	-34.765697	15.061136	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1146	41	40.194904	-34.590828	10.762484	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1147	41	37.009895	-36.114639	13.230972	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1148	41	37.022362	-37.278809	15.093244	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1149	41	37.281860	-36.977932	16.812386	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1150	41	36.010941	-35.645081	9.736654	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1151	41	35.875103	-35.703766	11.500031	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1152	41	36.892860	-34.345898	17.480757	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1153	41	34.852104	-36.491085	14.340549	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1154	41	32.948448	-33.123219	16.241329	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1155	41	36.020203	-33.585705	12.812077	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1156	41	36.506733	-33.566654	8.535584	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1157	41	35.860924	-29.845661	10.644500	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1158	41	33.140709	-31.762585	17.793591	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1159	41	34.253216	-31.068201	18.980762	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1160	41	34.556400	-32.249546	14.061342	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1161	41	36.275192	-32.085384	14.577629	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1162	41	31.073444	-34.421329	13.316997	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1163	41	32.001770	-33.126637	14.100664	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1164	41	35.464375	-32.184624	6.906415	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1165	41	37.257935	-32.039284	6.950205	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1166	41	34.964123	-32.370163	21.029644	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1167	41	31.755699	-33.726589	18.453646	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1168	41	34.127312	-33.851406	22.845070	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1169	41	30.926662	-35.205597	20.268415	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1170	41	32.103611	-35.272530	22.472422	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1171	41	34.084549	-30.118458	6.200377	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1172	41	38.363094	-30.397579	5.563556	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1173	41	33.945702	-28.344074	4.463370	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1174	41	38.216320	-28.617298	3.833578	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1175	41	36.009514	-27.586519	3.273998	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1176	41	36.963753	-30.203579	16.031332	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1177	41	32.884529	-30.490667	14.593350	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1178	41	36.257473	-28.470024	17.671049	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1179	41	32.186951	-28.760307	16.238529	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1180	41	33.869568	-27.744431	17.782145	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1181	41	30.280357	-32.177925	15.541884	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1182	41	30.921804	-36.464401	15.568175	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1183	41	28.743080	-32.402851	17.481997	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1184	41	29.387604	-36.679527	17.511179	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1185	41	28.291410	-34.650658	18.475124	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1186	41	47.869835	-36.585045	11.661585	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1187	41	47.456612	-34.915504	12.068846	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1188	41	45.156277	-33.953762	11.437436	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1189	41	46.030396	-38.181911	11.304239	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1190	41	41.935051	-36.819313	11.438818	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1191	41	42.299110	-40.508076	10.891459	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1192	41	41.790619	-38.904636	10.314969	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1193	41	39.591175	-39.273895	11.432402	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1194	41	43.246281	-39.274467	13.755857	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0



1195	41	39.430321	-38.828835	15.715108	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1196	41	37.357903	-40.504787	12.358402	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1197	41	37.307095	-38.825829	11.686153	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1198	41	42.944599	-37.700184	17.417212	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1199	41	42.073902	-36.900608	16.086174	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1200	41	34.867100	-38.836205	11.180478	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1201	41	36.273693	-39.693539	15.184975	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1202	41	32.141712	-38.693302	14.528502	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1203	41	40.948322	-35.490749	17.797581	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1204	41	40.435261	-39.786713	17.838287	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1205	41	37.704826	-37.260342	20.021879	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1206	41	30.587370	-37.654312	11.324800	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1207	41	31.147873	-37.235153	12.956574	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1208	41	36.971500	-35.020882	19.861135	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1209	41	38.130295	-35.296967	21.211920	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1210	41	32.038002	-39.174465	16.856503	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1211	41	32.851406	-37.593918	16.574015	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1212	41	36.943527	-39.274384	20.747961	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1213	41	36.378342	-39.097656	19.045967	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1214	41	31.073420	-40.632412	11.225861	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1215	41	29.375496	-38.137394	14.340281	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1216	41	29.775890	-42.572445	12.082734	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1217	41	28.087172	-40.082989	15.190016	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1218	41	28.281713	-42.307575	14.068199	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1219	41	36.050285	-41.178661	17.615177	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1220	41	36.697586	-41.404488	21.894917	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1221	41	35.127766	-43.489719	17.636545	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1222	41	35.774910	-43.714642	21.907789	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1223	41	34.986591	-44.765026	19.781834	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1224	41	37.988251	-32.585846	18.526556	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1225	41	37.835129	-33.530483	22.755816	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1226	41	37.896099	-30.166355	19.068287	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1227	41	37.750328	-31.106066	23.286623	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1228	41	37.776817	-29.413256	21.448450	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1229	41	34.162422	-36.503723	18.297655	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1230	41	32.616318	-40.500401	18.957657	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1231	41	34.764668	-36.343891	20.701078	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1232	41	33.217701	-40.328461	21.365416	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1233	41	34.291897	-38.250450	22.247225	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1234	41	51.808289	-38.849682	10.522525	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1235	41	52.326912	-40.571232	10.672541	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1236	41	53.567169	-40.993797	13.137667	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1237	41	53.503357	-37.269779	10.932396	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1238	41	56.635647	-38.040215	13.808193	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1239	41	55.245842	-41.473534	16.221119	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1240	41	53.893085	-40.524548	15.565575	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1241	41	55.739151	-34.372932	12.879030	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1242	41	55.481907	-35.674351	14.056793	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1243	41	56.435059	-40.604950	18.092365	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1244	41	54.323162	-37.852924	15.507530	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1245	41	56.324661	-36.392391	19.030617	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1246	41	57.452438	-36.215687	15.303843	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1247	41	57.901962	-34.777866	11.261011	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1248	41	61.398590	-35.676147	13.644725	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1249	41	58.447655	-37.240597	20.104191	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1250	41	56.883194	-37.168171	20.986458	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1251	41	58.742542	-37.754375	16.524084	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1252	41	58.749756	-36.106102	17.254086	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1253	41	54.863918	-34.488945	18.456011	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1254	41	56.460625	-34.645084	17.636084	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1255	41	62.281452	-34.210865	12.072380	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1256	41	62.230152	-35.873543	11.380253	1	"	X	"	"	21	0.00000	0.00000	"	"	H	"	"	1	0	0	1	H	0
1257	41	59.751221	-39.648392	20.653097	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1258	41	57.061237	-37.534138	23.312983	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1259	41	60.815773	-40.750843	22.613573	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1260	41	58.124062	-38.643299	25.264013	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0
1261	41	60.004559	-40.253979	24.925745	1	"	X	"	"	21	0.11346	0.11346	"	"	H	"	"	1	0	0	1	H	0

1262	41	61.635078	-36.022209	8.792278	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1263	41	63.170959	-32.453907	10.716531	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1264	41	62.401909	-35.157070	6.589144	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1265	41	63.931110	-31.597555	8.509958	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1266	41	63.550987	-32.944424	6.439627	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1267	41	60.522343	-39.396423	17.076027	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1268	41	60.511139	-35.451298	18.871002	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1269	41	62.193409	-40.151546	18.757154	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1270	41	62.172058	-36.218441	20.556568	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1271	41	63.021629	-38.567654	20.503637	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1272	41	57.060112	-33.253468	15.770931	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1273	41	52.962437	-33.304345	17.179413	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1274	41	56.526188	-31.325077	14.297049	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1275	41	52.435913	-31.369762	15.703970	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1276	41	54.214752	-30.375425	14.256988	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1277	41	47.080414	-36.049477	4.616873	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1278	41	47.892113	-34.567894	5.248399	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1279	41	48.237755	-38.315872	5.797021	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1280	41	47.674660	-34.435383	7.627697	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1281	41	47.917316	-37.974129	10.079088	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1282	41	47.563110	-41.516628	8.538100	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1283	41	46.436192	-40.174019	8.848165	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1284	41	50.102356	-40.108635	9.729950	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1285	41	46.079090	-40.697144	11.179515	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1286	41	49.321602	-40.105457	13.972630	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1287	41	46.028332	-40.620804	15.631193	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1288	41	47.726219	-41.052284	15.348559	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1289	41	49.049934	-39.413418	16.501532	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1290	41	45.571404	-38.072773	14.302567	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1291	41	48.195862	-35.202785	16.168278	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1292	41	50.509121	-35.150219	16.830105	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1293	41	49.289955	-35.329227	18.151184	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1294	41	46.994846	-33.788948	14.864869	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1295	41	45.242432	-33.626461	14.627978	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1296	41	51.270229	-33.734116	19.041451	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1297	41	51.538685	-38.035839	18.643866	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1298	41	54.036343	-35.967930	21.478556	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1299	41	47.444382	-32.778114	17.025009	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1300	41	44.034103	-35.405144	16.619907	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1301	41	45.155052	-33.904526	20.502693	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1302	41	53.843494	-32.392166	22.398710	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1303	41	53.776421	-34.133324	22.721558	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1304	41	47.789955	-31.431906	21.256405	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1305	41	46.084930	-31.919094	21.187571	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1306	41	54.329994	-39.646816	21.694889	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1307	41	54.910587	-37.971523	21.710775	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1308	41	42.466347	-36.457340	20.624250	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1309	41	44.154320	-36.021118	20.965149	1 " " X " "	21	0.00000	0.00000	" " H " "	"	1	0	0	1	H	0
1310	41	55.062748	-31.969721	19.846977	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1311	41	56.053173	-34.962543	22.823467	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1312	41	57.387970	-32.076523	18.973333	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1313	41	58.378067	-35.054596	21.947416	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1314	41	59.051735	-33.622391	20.015760	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
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1316	41	41.703705	-33.577000	19.439419	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1317	41	42.714306	-32.938560	24.286486	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1318	41	40.868088	-31.565186	20.626080	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1319	41	41.367569	-31.233046	23.049665	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
1320	41	49.296635	-33.887493	20.580593	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
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1322	41	49.935173	-35.911827	21.878935	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
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1326	41	51.451439	-39.546532	22.040619	1 " " X " "	21	0.11346	0.11346	" " H " "	"	1	0	0	1	H	0
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1329 41 50.669277 -37.657303 25.848108 1 " X " 21 0.11346 0.11346 " " H " " 1 0 0 1 H 0  
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