

Electronic Supplementary Material

**Canonical, Deprotonated, or Zwitterionic? II. A Computational Study  
on Amino Acid Interaction with the TiO<sub>2</sub> (110) Rutile Surface:  
Comparison with the Anatase (101) Surface**

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## Surface energies of TiO<sub>2</sub> (110) rutile and (101) anatase surfaces

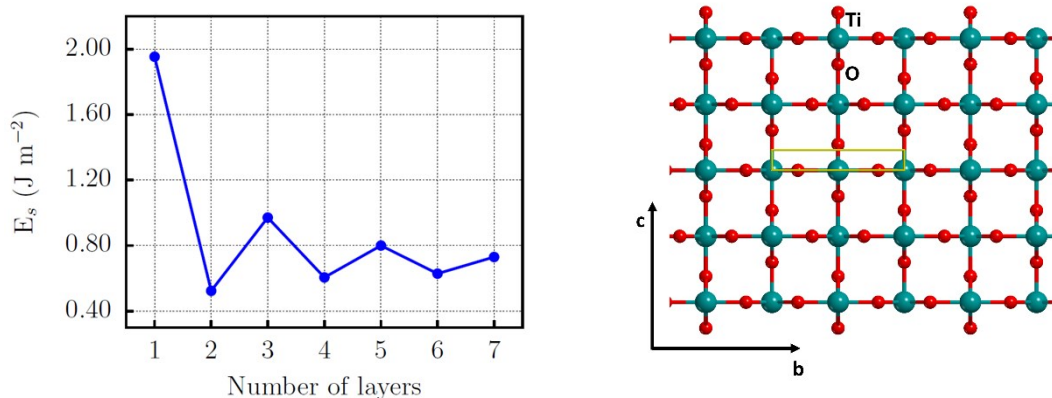
In order to choose the proper thickness of the surface, slab models from 1 up to 7 layers have been investigated (Figure S1) to identify the minimum thickness that leads to converged properties. To that purpose, the surface formation energy has been used as reference, following the equation:

$$E_S = \frac{E_n - nE_{bulk}}{2A}$$

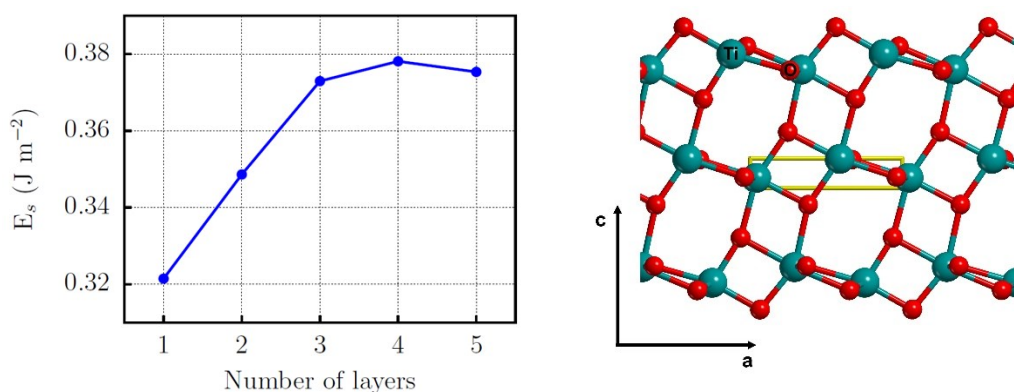
where  $E_n$  is the energy of the surface containing  $n$  layers,  $E_{bulk}$  is the energy of the bulk, and  $A$  is the area of the surface.

The TiO<sub>2</sub> (110) rutile has a higher surface formation energy than the (101) anatase one:  $E_S = 0.80 \text{ J m}^{-2}$  for a rutile 5-layer slab model and  $E_S = 0.37 \text{ J m}^{-2}$  for an anatase 3-layer slab model). The rutile (110) surface exhibits a slower convergence of the surface formation energy as a function of the slab thickness in comparison with the anatase one (see Figures S1 and S2). Accordingly, rutile (110) needs to use a larger number of layers than anatase (101) to reach well  $E_S$ -converged stable slab models.

The TiO<sub>2</sub> (110) rutile 5-layer slab model has been chosen for the amino acids adsorption because it represents the best compromise between the chemical accuracy and the computational cost.



**Figure S1.** Surface formation energy of the TiO<sub>2</sub> (110) rutile surface (left), and PBE-D2\* optimized structure (right).

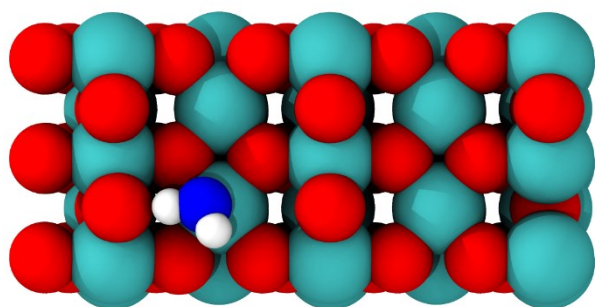


**Figure S2.** Surface formation energy of the  $\text{TiO}_2$  (101) anatase surface (left), and PBE-D2\* optimized structure (right).

Due to the oscillating behavior of the surface energy of the rutile (110) surfaces as a function of the number of layers, in a previous work we run some test calculations on the adsorption of a single water on  $\text{TiO}_2$  (110) rutile<sup>1</sup> from the 4-layer to the 7-layer surface models. Results are summarized in Table S1. The converged value seems to lay between the 4- and 5-layer models, with a percentage error around 10%. Moreover, we also run a test-case on the most stable adsorption mode of glycine on the 9-layer (110) rutile surface, and we obtain an adsorption energy of  $213.1 \text{ kJ mol}^{-1}$ , which, compared to the one obtained for the 5-layer model ( $238.3 \text{ kJ mol}^{-1}$ ), returns an error of about 10%, similar to that for the water case.

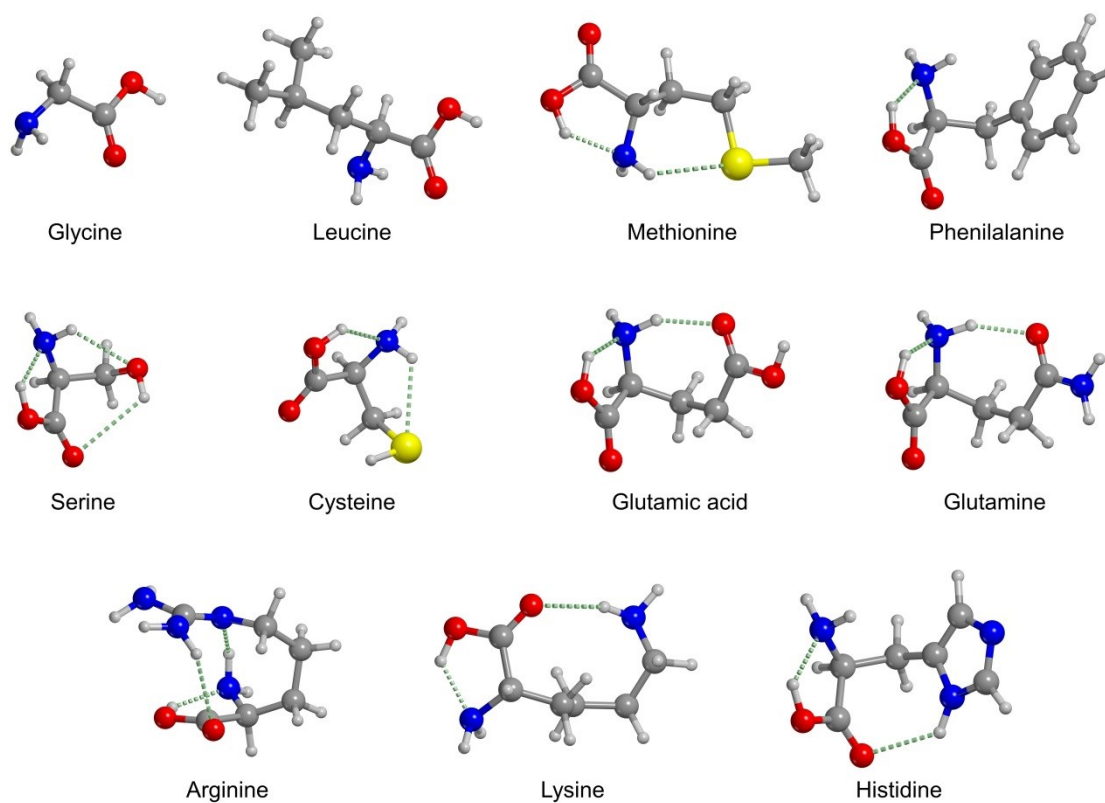
**Table S1.** Adsorption energies ( $\Delta E_{\text{ads}}$ ) of water adsorbed on  $\text{TiO}_2$  (110) rutile surface models of increasing thickness.

| Surface model | $\Delta E_{\text{ads}}$ (kJ/mol) |
|---------------|----------------------------------|
| 4 layer       | -86.9                            |
| 5 layer       | -105.6                           |
| 6 layer       | -89.8                            |
| 7 layer       | -95.0                            |



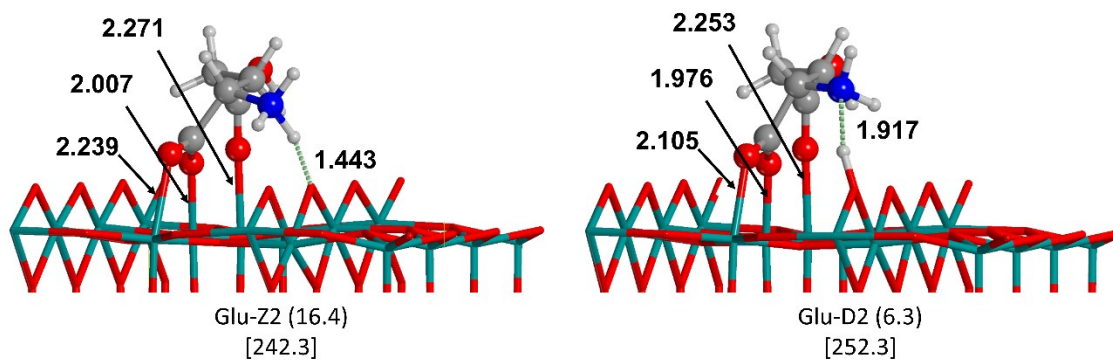
**Figure S3.** Water adsorbed on the  $\text{TiO}_2$  (110) rutile surface.

**Gas-phase amino acids in their corresponding most stable conformations**



**Figure S4.** PBE-D2\* optimized geometries for the studied amino acids in their most stable conformation in gas phase. Carbon in grey, oxygen in red, nitrogen in blue, sulfur in yellow, hydrogen in white.

### Glu/rutile complex with Ti-O dative lateral interactions



**Figure S5.** PBE-D2\* optimized geometries for glutamic acid (Glu) adsorbed on the  $\text{TiO}_2$  (110) rutile surface. Values in round and square parenthesis (in  $\text{kJ mol}^{-1}$ ) are the relative energies with respect to the most stable structure reported in the main text, and the adsorption energies, respectively. Bond distances are in Å.

## Optimized structures

In the following we report the optimized structures reported in the main text and in the ESI in POSCAR format.

### *Amino acids in gas phase*

GLY

```
1.000000000
 30.000000  0.000000  0.000000
 0.000000  30.000000  0.000000
 0.000000  0.000000  30.000000
H C N O
5 2 1 2
Cartesian
1.23265278 -1.00016301 0.87577303 #H
1.23265278 -1.00016301 -0.87577397 #H
-1.01355022 -1.90565901 -0.81540797 #H
-1.01355022 -1.90565901 0.81540703 #H
0.58987978 2.31726199 0.00000003 #H
0.57016378 -0.90761101 0.00000003 #C
0.01261978 0.51209999 0.00000003 #C
-0.40386022 -1.98072901 0.00000003 #N
-1.16813222 0.81468199 0.00000003 #O
1.01941578 1.43642099 0.00000003 #O
```

LEU

```
1.000000000
 30.000000  0.000000  0.000000
 0.000000  30.000000  0.000000
 0.000000  0.000000  30.000000
H C N O
13 6 1 2
Cartesian
-1.41249298 -0.47595831 1.83101461 #H
-2.59089401 -0.10543235 0.76641384 #H
-1.08258035 0.26799045 -0.98747782 #H
1.05959987 -0.23406850 1.14312093 #H
1.37769436 -0.04502744 -0.58692169 #H
0.09407164 2.08794677 1.19046368 #H
3.00532379 1.86557652 0.20317960 #H
2.32941623 3.23076089 1.11440147 #H
2.45983630 1.63233550 1.87830667 #H
-0.52108088 2.40390846 -1.20357165 #H
0.62220667 3.65589243 -0.70209192 #H
1.18982524 2.28474599 -1.67789579 #H
-0.15451268 -2.96178360 -1.70373313 #H
-0.72239357 -0.22382799 -0.07016536 #C
0.70972434 0.27709770 0.22901635 #C
-0.65838679 -1.72552700 -0.36058893 #C
0.82969073 1.79850004 0.42270121 #C
2.23193064 2.15001385 0.93464406 #C
0.50953341 2.57336669 -0.86039627 #C
```

-1.62700139 0.11282140 1.02218403 #N  
-0.95526402 -2.61126438 0.42496075 #O  
-0.19925367 -1.98545941 -1.62116409 #O

MET

1.000000000  
30.000000 0.000000 0.000000  
0.000000 30.000000 0.000000  
0.000000 0.000000 30.000000

H C N O S

11 5 1 2 1

Cartesian

-0.77110274 0.93830403 0.92258857 #H  
0.07305789 -0.54612381 -1.61245883 #H  
-0.26699325 1.18631437 -1.60592149 #H  
2.13409734 0.85552681 -1.38536072 #H  
1.49994571 1.57393644 0.11545785 #H  
4.40227890 0.19445553 -0.25687663 #H  
3.84397367 0.93868327 1.28128674 #H  
4.47991962 -0.72868094 1.26945979 #H  
-0.75913371 -1.88427282 0.17462065 #H  
-0.27890085 -1.17293794 1.56989683 #H  
-2.79799574 -0.91434064 0.78130735 #H  
-0.95862659 0.17506412 0.14658634 #C  
0.07545298 0.35334735 -0.97330869 #C  
1.49703797 0.66497016 -0.50808751 #C  
3.89707915 0.00720176 0.70099329 #C  
-2.38992468 0.49103519 -0.35950145 #C  
-0.98126040 -1.13244713 0.83066625 #N  
-2.64258639 1.37393762 -1.16007167 #O  
-3.33385556 -0.28295443 0.21245256 #O  
2.25316682 -0.69730665 0.44270602 #S

PHE

1.000000000  
30.000000 0.000000 0.000000  
0.000000 30.000000 0.000000  
0.000000 0.000000 30.000000

H C N O

11 9 1 2

Cartesian

-1.49385375 0.44629161 2.51267678 #H  
-1.54985578 -1.38262390 0.84188211 #H  
-2.47476297 0.05760861 0.36395642 #H  
0.73048049 -1.79860698 -0.27263902 #H  
-1.98148545 1.25248201 -1.65026500 #H  
1.97947238 -1.64770158 -2.41090460 #H  
-0.72421481 1.41383137 -3.78366934 #H  
1.09804913 1.45900686 2.24074238 #H  
-0.24578712 1.96859172 0.37151997 #H  
-1.19866373 2.48841959 1.61677189 #H  
1.26580026 -0.03734432 -4.17343310 #H  
-0.79330514 0.44732219 1.66177126 #C

|             |             |             |    |
|-------------|-------------|-------------|----|
| 0.46196384  | -0.27995560 | 2.20714079  | #C |
| -1.45857754 | -0.33907589 | 0.50836859  | #C |
| -0.70273103 | -0.26872962 | -0.79912727 | #C |
| 0.41561620  | -1.08723344 | -1.03765680 | #C |
| -1.09653246 | 0.62959575  | -1.80469404 | #C |
| 1.11685054  | -1.00111023 | -2.24185577 | #C |
| -0.39496837 | 0.71581637  | -3.01203860 | #C |
| 0.71746615  | -0.09828174 | -3.23191940 | #C |
| -0.44742014 | 1.84825817  | 1.36726460  | #N |
| 0.51978152  | -1.48582152 | 2.37566436  | #O |
| 1.46330220  | 0.56405023  | 2.51905845  | #O |

SER

|             |           |           |
|-------------|-----------|-----------|
| 1.000000000 |           |           |
| 30.000000   | 0.000000  | 0.000000  |
| 0.000000    | 30.000000 | 0.000000  |
| 0.000000    | 0.000000  | 30.000000 |

H C N O  
7 3 1 3

Cartesian

|             |             |             |    |
|-------------|-------------|-------------|----|
| -0.51485472 | 0.34502858  | 1.73602296  | #H |
| -0.63050391 | 1.87099001  | -0.58192304 | #H |
| -1.95096476 | -0.10972287 | -0.75983211 | #H |
| -2.52229145 | 0.49986058  | 0.66511075  | #H |
| 0.64982785  | -1.74917734 | 1.13532507  | #H |
| -1.12418934 | -1.98971058 | 1.14900121  | #H |
| 0.56560621  | -1.81248113 | -1.10241471 | #H |
| -0.49718532 | 0.02971314  | 0.67849341  | #C |
| 0.71347190  | 0.75871429  | 0.04758343  | #C |
| -0.29298078 | -1.48935474 | 0.62968825  | #C |
| -1.72810142 | 0.50702595  | 0.02661382  | #N |
| 1.86192156  | 0.36213198  | 0.15412836  | #O |
| 0.37264392  | 1.87815043  | -0.61759843 | #O |
| -0.31588345 | -1.97240663 | -0.71882970 | #O |

CYS

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|-------------|-----------|-----------|
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| 30.000000   | 0.000000  | 0.000000  |
| 0.000000    | 30.000000 | 0.000000  |
| 0.000000    | 0.000000  | 30.000000 |

H C N O S  
7 3 1 2 1

Cartesian

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|-------------|-------------|-------------|----|
| 0.82021658  | 0.83469577  | 1.69707002  | #H |
| 1.90534658  | 1.00827577  | -0.85418998 | #H |
| -0.33246342 | 1.82551577  | -0.78844998 | #H |
| 0.31093658  | 2.67892577  | 0.47742002  | #H |
| -0.96349342 | -0.88126423 | 1.55632002  | #H |
| -1.63004342 | 0.77129577  | 1.58175002  | #H |
| -1.35801342 | -1.32668423 | -0.92609998 | #H |
| 0.35594658  | 0.61663577  | 0.71850002  | #C |
| 1.26851658  | -0.46228423 | 0.08624002  | #C |
| -1.04774342 | 0.05297577  | 0.98779002  | #C |



|             |             |             |    |
|-------------|-------------|-------------|----|
| 0.41789658  | 1.83912577  | -0.08954998 | #N |
| 1.21284658  | -1.64224423 | 0.38292002  | #O |
| 2.15341658  | 0.03965577  | -0.79580998 | #O |
| -2.03933342 | -0.23580423 | -0.51264998 | #S |

GLU

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|-------------|-----------|-----------|--|
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| 0.000000    | 0.000000  | 30.000000 |  |

H C N O  
9 5 1 4

Cartesian

|             |             |             |    |
|-------------|-------------|-------------|----|
| -0.09850734 | 1.89939394  | 0.04525152  | #H |
| -3.61492734 | -0.02226606 | -1.12650848 | #H |
| 1.95656266  | 0.58388394  | 1.58013152  | #H |
| 0.43845266  | -1.08943606 | 2.07496152  | #H |
| -0.48795734 | 0.41467394  | 2.17595152  | #H |
| -0.54807734 | -1.52876606 | -0.22779848 | #H |
| -1.63513734 | -1.65961606 | 1.12766152  | #H |
| 1.20940266  | 2.53826394  | 0.83914152  | #H |
| 1.82259266  | 1.17996394  | -1.17404848 | #H |
| 1.18352266  | 0.45960394  | 0.80428152  | #C |
| 1.85815266  | -0.42780606 | -0.27249848 | #C |
| 0.00357266  | -0.27769606 | 1.47519152  | #C |
| -1.03933734 | -0.92969606 | 0.55799152  | #C |
| -2.01476734 | -0.00058606 | -0.11803848 | #C |
| 0.90610266  | 1.78719394  | 0.22269152  | #N |
| 2.08344266  | -1.61680606 | -0.11346848 | #O |
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GLN

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| 0.000000    | 0.000000  | 30.000000 |  |

H C N O  
10 5 2 3

Cartesian

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| -3.71346658 | -0.13689471 | -1.27677105 | #H |
| 1.95144342  | 0.70740529  | 1.50567895  | #H |
| 0.45390342  | -0.93819471 | 2.14362895  | #H |
| -0.48746658 | 0.56236529  | 2.13446895  | #H |
| -0.54279658 | -1.55169471 | -0.10988105 | #H |
| -1.61800658 | -1.58436471 | 1.27339895  | #H |
| 1.20313342  | 2.58465529  | 0.59514895  | #H |
| 1.71881342  | 1.06104529  | -1.30576105 | #H |
| 1.17209342  | 0.51387529  | 0.75067895  | #C |
| 1.84062342  | -0.45220471 | -0.25869105 | #C |

|             |             |             |    |
|-------------|-------------|-------------|----|
| 0.00508342  | -0.17915471 | 1.48737895  | #C |
| -1.04144658 | -0.90062471 | 0.62788895  | #C |
| -2.04040658 | -0.00963471 | -0.09890105 | #C |
| 0.86186342  | 1.78397529  | 0.06667895  | #N |
| -3.04494658 | -0.67293471 | -0.73617105 | #N |
| 2.11565342  | -1.61261471 | 0.00244895  | #O |
| -1.97880658 | 1.22838529  | -0.11441105 | #O |
| 2.09145342  | 0.12621529  | -1.44513105 | #O |

ARG

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|-------------|-----------|-----------|
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| 0.000000    | 0.000000  | 30.000000 |

H C N O  
14 6 4 2

Cartesian

|             |             |             |    |
|-------------|-------------|-------------|----|
| -1.96933393 | -2.23275908 | -0.02639639 | #H |
| 0.54351713  | -2.18132394 | 0.70603047  | #H |
| -1.62269684 | -1.71772153 | 2.21665560  | #H |
| -0.52368710 | -0.50800229 | 1.84796014  | #H |
| -2.49498531 | -0.08208636 | -1.20500927 | #H |
| -3.38020269 | -0.41125722 | 0.28675292  | #H |
| -2.81995133 | 1.94843280  | 0.11299783  | #H |
| -2.05729120 | 1.25465261  | 1.54108136  | #H |
| -0.59356138 | 1.70619415  | -1.10221609 | #H |
| -0.65640201 | 2.90217570  | 0.20203016  | #H |
| 2.37487531  | 0.50082347  | 1.95491626  | #H |
| 2.88185102  | 1.21801624  | -1.37323684 | #H |
| 3.30406344  | 0.05669238  | 0.61150900  | #H |
| 1.23812693  | 1.19520553  | -1.79316696 | #H |
| -1.42338126 | -1.29558327 | 0.19031631  | #C |
| -0.21707243 | -1.36278440 | -0.77297192 | #C |
| -2.38977664 | -0.13400887 | -0.10997502 | #C |
| -2.02830341 | 1.25453049  | 0.43849885  | #C |
| -0.67347909 | 1.81526371  | -0.00372527 | #C |
| 1.59211379  | 1.10576795  | 0.21076718  | #C |
| -0.90062420 | -1.42179192 | 1.56111902  | #N |
| 0.41087946  | 1.18323601  | 0.73676277  | #N |
| 2.67107877  | 0.74360406  | 1.01379652  | #N |
| 1.93276559  | 1.43434825  | -1.08983555 | #N |
| 0.82714574  | -2.04240590 | -0.24843883 | #O |
| -0.20635674 | -0.92371912 | -1.91206944 | #O |

LYS

|             |           |           |
|-------------|-----------|-----------|
| 1.000000000 |           |           |
| 30.000000   | 0.000000  | 0.000000  |
| 0.000000    | 30.000000 | 0.000000  |
| 0.000000    | 0.000000  | 30.000000 |

H C N O  
14 6 2 2

Cartesian

|            |             |            |    |
|------------|-------------|------------|----|
| 3.08765780 | -0.04332680 | 0.09379304 | #H |
|------------|-------------|------------|----|

|             |             |             |    |
|-------------|-------------|-------------|----|
| 1.44333352  | -0.18002454 | -2.11247901 | #H |
| 2.40789998  | -2.09831930 | -1.43193676 | #H |
| 1.79728360  | -2.05455012 | 0.09511113  | #H |
| -0.49019145 | -1.62590488 | -1.68876893 | #H |
| -0.83969653 | 0.07064217  | -1.34285070 | #H |
| -0.33138147 | -0.48413372 | 1.16535031  | #H |
| -0.38256753 | -2.18363943 | 0.69848233  | #H |
| -2.52184497 | -1.54990215 | 1.60411031  | #H |
| -2.74479202 | -1.87921104 | -0.12335102 | #H |
| -2.89047500 | 0.51062011  | -0.63682759 | #H |
| -4.01023976 | 0.09871828  | 0.66363246  | #H |
| -2.97851976 | 1.99398420  | 1.43563107  | #H |
| -1.47122835 | 1.53882586  | 0.99319355  | #H |
| -2.93985756 | 0.20001953  | 0.42691711  | #C |
| -2.28486812 | -1.17872492 | 0.59490893  | #C |
| -0.75826695 | -1.18244396 | 0.42634254  | #C |
| -0.28172530 | -0.80549050 | -0.98301840 | #C |
| 1.20665503  | -0.44020638 | -1.06630358 | #C |
| 1.50554975  | 0.85724278  | -0.27605005 | #C |
| -2.36305574 | 1.18561449  | 1.34890668  | #N |
| 2.17556186  | -1.47736064 | -0.65824233 | #N |
| 2.72718473  | 0.87066196  | 0.29228768  | #O |
| 0.72916777  | 1.79562546  | -0.20142381 | #O |

HIS

1.000000000

30.000000 0.000000 0.000000

0.000000 30.000000 0.000000

0.000000 0.000000 30.000000

H C N O

9 6 3 2

Cartesian

|             |             |             |    |
|-------------|-------------|-------------|----|
| -0.66485541 | -1.71827554 | 0.46332648  | #H |
| 2.25820459  | 1.18542446  | 1.10218648  | #H |
| 0.29358459  | 0.21885446  | 2.17010648  | #H |
| -0.05019541 | 1.86675446  | 1.62325648  | #H |
| -2.34657541 | 2.10887446  | 0.00139648  | #H |
| -2.88382541 | -1.97074554 | -0.82705352 | #H |
| 2.43844459  | 0.28827446  | -1.46171352 | #H |
| 0.51497459  | 1.66843446  | -1.18919352 | #H |
| 1.69173459  | 2.63436446  | -0.55282352 | #H |
| 1.44020459  | 0.83169446  | 0.45162648  | #C |
| 0.13298459  | 0.83991446  | 1.27597648  | #C |
| -1.06552541 | 0.37226446  | 0.51896648  | #C |
| -2.14255541 | 1.04159446  | -0.03547352 | #C |
| -2.47224541 | -1.03009554 | -0.47321352 | #C |
| 1.84944459  | -0.60456554 | 0.04904648  | #C |
| -1.29902541 | -0.95965554 | 0.22418648  | #N |
| -3.01196541 | 0.16458446  | -0.64782352 | #N |
| 1.44475459  | 1.66745446  | -0.75864352 | #N |
| 2.50272459  | -0.65685554 | -1.12347352 | #O |
| 1.62256459  | -1.59179554 | 0.73326648  | #O |

*Amino acids adsorbed on rutile*

Rut-Gly\_D1

1.000000000

|          |           |           |
|----------|-----------|-----------|
| 8.876100 | 0.000000  | 0.000000  |
| 0.000000 | 12.992946 | 0.000000  |
| 0.000000 | 0.000000  | 30.000000 |

H C N O Ti

5 2 1 122 60

Cartesian

|            |            |             |    |
|------------|------------|-------------|----|
| 6.34353000 | 4.49238572 | 6.22099473  | #H |
| 4.54671000 | 4.55578572 | 6.26435473  | #H |
| 6.50854000 | 6.67735572 | 4.03966473  | #H |
| 4.68280000 | 6.58925572 | 4.93835473  | #H |
| 5.72964000 | 6.79057572 | 6.21386473  | #H |
| 5.39936000 | 4.10388572 | 4.33245473  | #C |
| 5.44329000 | 4.80895572 | 5.67931473  | #C |
| 5.55629000 | 6.25193572 | 5.36445473  | #N |
| 6.52075000 | 3.87635572 | 3.76789473  | #O |
| 4.25456000 | 3.90537572 | 3.80455473  | #O |
| 0.91942000 | 0.49472572 | 3.02259473  | #O |
| 2.36939000 | 4.99934572 | 1.87075473  | #O |
| 2.38143000 | 2.52746572 | 1.87366473  | #O |
| 0.92170000 | 0.48745572 | 0.44272473  | #O |
| 0.91964000 | 3.75822572 | 29.72058473 | #O |
| 2.39625000 | 1.79578572 | 28.45205473 | #O |
| 2.38663000 | 5.72732572 | 28.47098473 | #O |
| 0.91754000 | 3.76850572 | 27.17064473 | #O |
| 0.92359000 | 0.50186572 | 26.45622473 | #O |
| 2.40171000 | 5.01794572 | 25.16305473 | #O |
| 2.39957000 | 2.50856572 | 25.17026473 | #O |
| 0.92460000 | 0.50919572 | 23.85340473 | #O |
| 0.91589000 | 3.77367572 | 23.16843473 | #O |
| 2.39647000 | 1.81220572 | 21.86412473 | #O |
| 2.39626000 | 5.71685572 | 21.83127473 | #O |
| 0.91345000 | 3.76306572 | 20.59192473 | #O |
| 0.91558000 | 0.50483572 | 19.87885473 | #O |
| 2.39298000 | 4.98224572 | 18.41971473 | #O |
| 2.39150000 | 2.54133572 | 18.44116473 | #O |
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| 3.88705000 | 0.52900572 | 3.01147473  | #O |
| 5.36076000 | 5.02121572 | 1.64070473  | #O |
| 5.35339000 | 2.49372572 | 1.70534473  | #O |
| 3.86125000 | 0.45399572 | 0.43165473  | #O |
| 3.83501000 | 3.75206572 | 29.76698473 | #O |
| 5.35826000 | 1.79478572 | 28.49167473 | #O |
| 5.35267000 | 5.72751572 | 28.50760473 | #O |
| 3.90233000 | 3.76946572 | 27.19539473 | #O |
| 3.88560000 | 0.50221572 | 26.45828473 | #O |
| 5.34930000 | 5.02033572 | 25.16238473 | #O |
| 5.35410000 | 2.50880572 | 25.16263473 | #O |
| 3.88521000 | 0.50588572 | 23.85226473 | #O |
| 3.87292000 | 3.77218572 | 23.16961473 | #O |
| 5.35584000 | 1.81099572 | 21.86331473 | #O |
| 5.35146000 | 5.71583572 | 21.83338473 | #O |
| 3.87293000 | 3.75947572 | 20.59094473 | #O |

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|------------|-------------|-------------|----|
| 3.87632000 | 0.50529572  | 19.87762473 | #O |
| 5.35072000 | 4.98287572  | 18.42147473 | #O |
| 5.35111000 | 2.54147572  | 18.43972473 | #O |
| 3.86922000 | 0.51542572  | 17.29583473 | #O |
| 6.82812000 | 0.53361572  | 3.01123473  | #O |
| 8.34197000 | 5.00390572  | 1.84692473  | #O |
| 8.34050000 | 2.52675572  | 1.86164473  | #O |
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| 6.87335000 | 3.74949572  | 29.75803473 | #O |
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| 8.31664000 | 5.72697572  | 28.47969473 | #O |
| 6.80738000 | 3.76840572  | 27.19050473 | #O |
| 6.84244000 | 0.50430572  | 26.45914473 | #O |
| 8.30830000 | 5.01506572  | 25.16464473 | #O |
| 8.30974000 | 2.50986572  | 25.16711473 | #O |
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| 0.91886000 | 10.23775572 | 29.75214473 | #O |
| 2.38612000 | 8.30134572  | 28.45295473 | #O |
| 2.39500000 | 12.18629572 | 28.44642473 | #O |
| 0.91658000 | 10.24346572 | 27.16078473 | #O |
| 0.92081000 | 7.00690572  | 26.42367473 | #O |
| 2.39518000 | 11.49879572 | 25.15369473 | #O |
| 2.39924000 | 8.99238572  | 25.15176473 | #O |
| 0.91768000 | 7.00592572  | 23.83852473 | #O |
| 0.91557000 | 10.24078572 | 23.14823473 | #O |
| 2.39722000 | 8.30583572  | 21.82553473 | #O |
| 2.39595000 | 12.19928572 | 21.85944473 | #O |
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| 2.39314000 | 9.03066572  | 18.39904473 | #O |
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| 5.35524000 | 11.49893572 | 25.15582473 | #O |
| 5.34864000 | 8.99324572  | 25.15519473 | #O |

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| 3.87508000 | 7.00797572  | 23.84349473 | #O  |
| 3.87246000 | 10.24370572 | 23.14860473 | #O  |
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| 3.87258000 | 10.25635572 | 20.56790473 | #O  |
| 3.87280000 | 7.01090572  | 19.82187473 | #O  |
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| 6.84816000 | 7.07844572  | 0.47000473  | #O  |
| 6.83497000 | 10.24262572 | 29.74301473 | #O  |
| 8.32076000 | 8.30508572  | 28.45967473 | #O  |
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| 6.83573000 | 10.24101572 | 27.16067473 | #O  |
| 6.83155000 | 7.00754572  | 26.45517473 | #O  |
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| 0.91424000 | 0.51958572  | 21.74883473 | #Ti |
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| 0.91218000 | 3.76069572  | 18.78529473 | #Ti |
| 2.38736000 | 0.51487572  | 18.38584473 | #Ti |
| 3.88423000 | 3.73136572  | 1.78137473  | #Ti |
| 5.35690000 | 0.48883572  | 1.91147473  | #Ti |
| 3.87832000 | 0.51830572  | 28.57083473 | #Ti |
| 5.34950000 | 3.77560572  | 28.59698473 | #Ti |
| 3.86473000 | 3.76266572  | 25.25017473 | #Ti |
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| 6.84624000 | 3.74495572  | 1.75249473  | #Ti |
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| 6.83266000 | 0.51416572  | 28.57094473 | #Ti |
| 8.27160000 | 3.77088572  | 28.38120473 | #Ti |
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| 8.17459000 | 0.51510572  | 25.15829473 | #Ti |

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|------------|-------------|-------------|-----|
| 6.82284000 | 0.51715572  | 21.74736473 | #Ti |
| 8.30729000 | 3.75837572  | 21.98937473 | #Ti |
| 6.82965000 | 3.76013572  | 18.78493473 | #Ti |
| 8.30506000 | 0.51428572  | 18.38632473 | #Ti |
| 0.91683000 | 10.25480572 | 1.56934473  | #Ti |
| 2.44593000 | 7.00000572  | 1.97890473  | #Ti |
| 0.93259000 | 7.01296572  | 28.65540473 | #Ti |
| 2.39139000 | 10.27740572 | 28.36874473 | #Ti |
| 0.89254000 | 10.25258572 | 25.16003473 | #Ti |
| 2.31107000 | 6.99593572  | 25.02643473 | #Ti |
| 0.90639000 | 7.01161572  | 21.68568473 | #Ti |
| 2.39174000 | 10.26109572 | 21.94953473 | #Ti |
| 0.91224000 | 10.25268572 | 18.75505473 | #Ti |
| 2.38637000 | 7.00172572  | 18.32308473 | #Ti |
| 3.87571000 | 10.24013572 | 1.55999473  | #Ti |
| 5.25539000 | 6.98946572  | 1.65711473  | #Ti |
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| 8.30877000 | 10.26965572 | 21.95004473 | #Ti |
| 6.82957000 | 10.25282572 | 18.75395473 | #Ti |
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Rut-Gly\_D2

1.000000000

|          |           |           |
|----------|-----------|-----------|
| 8.876100 | 0.000000  | 0.000000  |
| 0.000000 | 12.992946 | 0.000000  |
| 0.000000 | 0.000000  | 30.000000 |

H C N O Ti

5 2 1 122 60

Cartesian

|            |            |            |    |
|------------|------------|------------|----|
| 6.16795000 | 5.56488912 | 5.71882641 | #H |
| 5.16502000 | 4.26413912 | 6.41353641 | #H |
| 3.21286000 | 5.44110912 | 5.60716641 | #H |
| 4.14069000 | 6.58941912 | 6.34095641 | #H |
| 3.96441000 | 6.70557912 | 4.02068641 | #H |
| 5.30532000 | 4.25763912 | 4.27536641 | #C |
| 5.23401000 | 5.00469912 | 5.59523641 | #C |
| 4.09890000 | 5.94694912 | 5.54855641 | #N |
| 6.44933000 | 4.00816912 | 3.77441641 | #O |
| 4.18354000 | 3.98690912 | 3.72955641 | #O |
| 0.90505000 | 0.59174912 | 2.99484641 | #O |

|            |            |             |    |
|------------|------------|-------------|----|
| 2.35515000 | 5.09843912 | 1.81138641  | #O |
| 2.35922000 | 2.62301912 | 1.83618641  | #O |
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| 0.90526000 | 3.84749912 | 29.68592641 | #O |
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| 2.38700000 | 5.81978912 | 28.44680641 | #O |
| 0.90348000 | 3.85811912 | 27.13823641 | #O |
| 0.91760000 | 0.60055912 | 26.42264641 | #O |
| 2.39162000 | 5.11182912 | 25.13771641 | #O |
| 2.39313000 | 2.60648912 | 25.13451641 | #O |
| 0.92226000 | 0.60574912 | 23.81762641 | #O |
| 0.91045000 | 3.87099912 | 23.13754641 | #O |
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| 2.39341000 | 2.64205912 | 18.40753641 | #O |
| 0.91140000 | 0.61753912 | 17.26250641 | #O |
| 3.87261000 | 0.62884912 | 2.98329641  | #O |
| 5.33696000 | 5.11413912 | 1.60880641  | #O |
| 5.34507000 | 2.58645912 | 1.67018641  | #O |
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| 5.34823000 | 5.82162912 | 28.47731641 | #O |
| 3.89605000 | 3.86048912 | 27.15950641 | #O |
| 3.87923000 | 0.60120912 | 26.42541641 | #O |
| 5.34972000 | 5.11729912 | 25.13197641 | #O |
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| 3.87242000 | 0.60514912 | 19.84265641 | #O |
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| 5.34916000 | 2.64173912 | 18.40502641 | #O |
| 3.87027000 | 0.61557912 | 17.26003641 | #O |
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| 8.33116000 | 5.09366912 | 1.83377641  | #O |
| 8.31777000 | 2.62208912 | 1.84342641  | #O |
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| 8.31433000 | 5.82054912 | 28.44556641 | #O |
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| 8.31209000 | 1.91061912 | 21.82855641 | #O |
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| 6.83283000 | 0.60857912  | 19.84123641 | #O |
| 8.30817000 | 5.08293912  | 18.39545641 | #O |
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| 6.82938000 | 0.61589912  | 17.26108641 | #O |
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| 2.38645000 | 11.55713912 | 1.88592641  | #O |
| 2.38601000 | 9.12384912  | 1.90415641  | #O |
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| 0.90434000 | 7.10572912  | 26.40870641 | #O |
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| 2.38902000 | 9.09490912  | 25.11770641 | #O |
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| 0.90799000 | 10.34648912 | 23.11634641 | #O |
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| 2.39452000 | 12.29740912 | 21.82437641 | #O |
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| 5.34674000 | 11.55198912 | 1.88414641  | #O |
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H C N O Ti

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H C N O Ti

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Rut-Gly-D4

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H C N O Ti

5 2 1 122 60

Cartesian

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| 3.87720000 | 4.06847000  | 15.41935000 | #Ti |
| 5.24711000 | 0.80947000  | 15.31291000 | #Ti |
| 3.88205000 | 0.78086000  | 11.89275000 | #Ti |
| 5.35492000 | 4.02715000  | 12.22777000 | #Ti |
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| 6.83940000 | 0.78002000  | 5.29503000  | #Ti |
| 8.31047000 | 4.03191000  | 5.60548000  | #Ti |
| 6.83588000 | 4.03391000  | 2.39918000  | #Ti |
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| 2.40402000 | 7.30303000  | 15.53102000 | #Ti |
| 0.90920000 | 7.28325000  | 12.17614000 | #Ti |
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| 6.82929000 | 7.27159000  | 5.34481000  | #Ti |
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Rut-Gly-D5

1.000000000

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| 0.000000 | 0.000000  | 30.000000 |

H C N O Ti

5 2 1 122 60

Cartesian

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| 6.80497000 | 6.74219000 | 17.56527000 | #H |
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Rut-Gly-C

1.000000000

8.876100 0.000000 0.000000

0.000000 12.992946 0.000000

0.000000 0.000000 30.000000

H C N O Ti

5 2 1 122 60

Cartesian

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H C N O Ti

13 6 1 162 80

Cartesian

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H C N O Ti

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Rut-Leu-C

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H C N O Ti

13 6 1 162 80

Cartesian

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Rut-Met-D

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0.000000 0.000000 30.000000

H C N O S Ti

11 5 1 162 1 80

Cartesian

|            |            |             |    |
|------------|------------|-------------|----|
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| 3.71278000 | 0.78216000  | 12.20242000 | #Ti |
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| 0.75072000 | 10.51540000 | 2.38442000  | #Ti |
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Rut-Met-Z

1.000000000

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| 0.000000  | 12.992946 | 0.000000  |
| 0.000000  | 0.000000  | 30.000000 |

H C N O S Ti

11 5 1 162 1 80

Cartesian

|            |            |             |    |
|------------|------------|-------------|----|
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H C N O S Ti

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Rut-Ser-D

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H C N O Ti

7 3 1 123 60

Cartesian

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Rut-Ser-Z

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H C N O Ti

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Cartesian

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Rut-Ser-C

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H C N O Ti

7 3 1 123 60

Cartesian

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Rut-Cys-D

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H C N O S Ti

7 3 1 122 1 60

Cartesian

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H C N O S Ti

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Cartesian

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| 6.83237000 | 7.27329000  | 3.45904000  | #O  |
| 8.31491000 | 11.73294000 | 2.02935000  | #O  |
| 8.31450000 | 9.29389000  | 2.03076000  | #O  |
| 6.83648000 | 7.26839000  | 0.87314000  | #O  |
| 6.80731000 | 3.03968000  | 20.51598000 | #S  |
| 0.92472000 | 4.03789000  | 15.10795000 | #Ti |
| 2.39763000 | 0.76624000  | 15.53588000 | #Ti |
| 0.91289000 | 0.81409000  | 12.17548000 | #Ti |
| 2.43259000 | 4.05976000  | 11.97940000 | #Ti |
| 0.88680000 | 4.01967000  | 8.81111000  | #Ti |
| 2.25743000 | 0.78222000  | 8.76698000  | #Ti |
| 0.91712000 | 0.79739000  | 5.35958000  | #Ti |
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| 0.91710000 | 4.02384000  | 2.39077000  | #Ti |
| 2.39209000 | 0.77657000  | 1.99812000  | #Ti |
| 3.88384000 | 3.99199000  | 15.31379000 | #Ti |
| 5.35969000 | 0.75351000  | 15.51713000 | #Ti |
| 3.87622000 | 0.80802000  | 12.17892000 | #Ti |
| 5.35176000 | 4.07739000  | 12.15021000 | #Ti |
| 3.85035000 | 4.03383000  | 8.83243000  | #Ti |
| 5.21491000 | 0.77961000  | 8.76584000  | #Ti |
| 3.87357000 | 0.79546000  | 5.36008000  | #Ti |
| 5.35327000 | 4.05117000  | 5.59710000  | #Ti |
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| 5.35005000 | 0.77618000  | 1.99707000  | #Ti |
| 6.84639000 | 4.00021000  | 15.28580000 | #Ti |
| 8.32058000 | 0.76925000  | 15.53283000 | #Ti |
| 6.83640000 | 0.81728000  | 12.17771000 | #Ti |
| 8.28293000 | 4.08076000  | 11.96966000 | #Ti |
| 6.79777000 | 4.02508000  | 8.83307000  | #Ti |
| 8.17388000 | 0.78094000  | 8.76658000  | #Ti |
| 6.82547000 | 0.79523000  | 5.35942000  | #Ti |
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| 2.40860000 | 7.25914000  | 15.59805000 | #Ti |
| 0.93878000 | 7.30476000  | 12.28587000 | #Ti |
| 2.39255000 | 10.56775000 | 11.97732000 | #Ti |
| 0.87276000 | 10.52164000 | 8.77576000  | #Ti |
| 2.28701000 | 7.26894000  | 8.67196000  | #Ti |
| 0.90945000 | 7.29085000  | 5.31950000  | #Ti |
| 2.39349000 | 10.54298000 | 5.56826000  | #Ti |
| 0.91732000 | 10.51830000 | 2.37532000  | #Ti |

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| 3.88117000 | 10.50315000 | 15.16766000 | #Ti |
| 5.27509000 | 7.25909000  | 15.27452000 | #Ti |
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| 5.35348000 | 10.57007000 | 11.97250000 | #Ti |
| 3.83055000 | 10.51906000 | 8.77703000  | #Ti |
| 5.34318000 | 7.27352000  | 8.61106000  | #Ti |
| 3.87187000 | 7.29074000  | 5.29697000  | #Ti |
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| 8.27961000 | 7.26187000  | 15.63002000 | #Ti |
| 6.84471000 | 7.32811000  | 12.16089000 | #Ti |
| 8.31458000 | 10.56545000 | 11.97436000 | #Ti |
| 6.79118000 | 10.52083000 | 8.77469000  | #Ti |
| 8.26993000 | 7.26666000  | 8.88248000  | #Ti |
| 6.84044000 | 7.28838000  | 5.31304000  | #Ti |
| 8.31065000 | 10.55167000 | 5.56999000  | #Ti |
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| 8.31280000 | 7.26689000  | 1.96416000  | #Ti |

Rut-Cys-C

1.000000000

|          |           |           |
|----------|-----------|-----------|
| 8.876100 | 0.000000  | 0.000000  |
| 0.000000 | 12.992946 | 0.000000  |
| 0.000000 | 0.000000  | 30.000000 |

H C N O S Ti

7 3 1 122 1 60

Cartesian

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| 3.95694000 | 2.81918000 | 17.64522000 | #H |
| 2.62823000 | 2.61878000 | 20.95304000 | #H |
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| 3.11728000 | 5.46288000 | 18.66143000 | #H |
| 5.49335000 | 5.61580000 | 19.57429000 | #H |
| 5.18879000 | 6.08633000 | 17.88110000 | #H |
| 3.82577000 | 4.61583000 | 18.69561000 | #C |
| 3.62555000 | 3.97761000 | 20.08260000 | #C |
| 5.20934000 | 5.25197000 | 18.57953000 | #C |
| 3.46030000 | 3.71951000 | 17.57492000 | #N |
| 4.15261000 | 4.37153000 | 21.10324000 | #O |
| 2.73398000 | 2.94761000 | 20.03576000 | #O |
| 6.51605000 | 0.88711000 | 16.61186000 | #O |
| 8.02249000 | 5.35346000 | 15.45224000 | #O |
| 8.02308000 | 2.88966000 | 15.47839000 | #O |
| 6.53316000 | 0.83184000 | 14.03811000 | #O |
| 6.53898000 | 4.12816000 | 13.36836000 | #O |
| 8.00088000 | 2.16383000 | 12.06184000 | #O |
| 6.49052000 | 4.11475000 | 10.78717000 | #O |
| 6.52875000 | 0.86941000 | 10.06747000 | #O |
| 7.99452000 | 5.36778000 | 8.77154000  | #O |
| 7.99722000 | 2.86137000 | 8.77189000  | #O |
| 6.52584000 | 0.86488000 | 7.45883000  | #O |

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| 7.99998000 | 2.16038000  | 5.46499000  | #O |
| 8.00008000 | 6.05948000  | 5.45953000  | #O |
| 6.52153000 | 4.11042000  | 4.19996000  | #O |
| 6.52009000 | 0.86400000  | 3.47437000  | #O |
| 8.00214000 | 5.33519000  | 2.04185000  | #O |
| 8.00215000 | 2.89611000  | 2.04227000  | #O |
| 6.52376000 | 0.87170000  | 0.89266000  | #O |
| 0.61595000 | 0.87680000  | 16.61971000 | #O |
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| 2.03767000 | 2.86905000  | 15.39640000 | #O |
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| 0.59802000 | 4.13275000  | 13.30269000 | #O |
| 2.08254000 | 2.16071000  | 12.06604000 | #O |
| 2.08396000 | 6.07473000  | 12.05297000 | #O |
| 0.60359000 | 4.11557000  | 10.76746000 | #O |
| 0.61028000 | 0.86434000  | 10.06314000 | #O |
| 2.08458000 | 5.37003000  | 8.77272000  | #O |
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| 6.52948000 | 7.37085000  | 10.06761000 | #O |
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| 7.99946000 | 9.35714000  | 8.75860000  | #O |
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| 6.52046000 | 10.60571000 | 6.75561000  | #O |
| 8.00020000 | 8.66001000  | 5.45822000  | #O |
| 8.00075000 | 12.55255000 | 5.45809000  | #O |
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| 8.00189000 | 9.39188000  | 2.01955000  | #O |
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| 2.08594000 | 9.39866000  | 15.50521000 | #O |
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| 2.08002000 | 12.55411000 | 12.04499000 | #O |
| 0.60169000 | 10.61006000 | 10.75925000 | #O |
| 0.61169000 | 7.37034000  | 10.06361000 | #O |
| 2.08173000 | 11.86484000 | 8.75787000  | #O |
| 2.08258000 | 9.35836000  | 8.76000000  | #O |
| 0.60656000 | 7.36033000  | 7.45709000  | #O |
| 0.60315000 | 10.60593000 | 6.75484000  | #O |
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| 2.08230000 | 12.55205000 | 5.45524000  | #O |
| 0.60248000 | 10.60641000 | 4.17880000  | #O |
| 0.60452000 | 7.36367000  | 3.47158000  | #O |
| 2.08497000 | 11.83211000 | 2.02709000  | #O |
| 2.08443000 | 9.39205000  | 2.02326000  | #O |
| 0.60584000 | 7.35755000  | 0.88854000  | #O |
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| 5.04214000 | 11.83009000 | 15.51414000 | #O |
| 5.04210000 | 9.40241000  | 15.49737000 | #O |
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| 3.56154000 | 10.62003000 | 13.33813000 | #O |
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| 3.56096000 | 10.61238000 | 10.75982000 | #O |
| 3.57405000 | 7.36785000  | 10.06532000 | #O |
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| 5.03945000 | 9.35765000  | 8.75769000  | #O |
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| 3.55980000 | 10.60763000 | 6.75498000  | #O |
| 5.04356000 | 8.66012000  | 5.45656000  | #O |
| 5.04120000 | 12.55270000 | 5.45921000  | #O |
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| 3.56375000 | 7.36625000  | 3.47085000  | #O |
| 5.04400000 | 11.83055000 | 2.02270000  | #O |
| 5.04407000 | 9.39104000  | 2.02225000  | #O |
| 3.56394000 | 7.35908000  | 0.88790000  | #O |
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| 6.51256000 | 4.07847000  | 18.03353000 | #S |

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| 7.99373000 | 4.07329000  | 5.58555000  | #Ti |
| 6.52243000 | 4.11478000  | 2.38924000  | #Ti |
| 8.00309000 | 0.87072000  | 1.97999000  | #Ti |
| 0.59969000 | 4.11637000  | 15.09521000 | #Ti |
| 2.08531000 | 0.86915000  | 15.50614000 | #Ti |
| 0.59721000 | 0.87510000  | 12.16154000 | #Ti |
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| 0.55675000 | 4.11570000  | 8.79838000  | #Ti |
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| 2.08135000 | 4.07321000  | 5.58334000  | #Ti |
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| 7.99618000 | 10.62266000 | 11.95892000 | #Ti |
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| 7.99517000 | 10.56985000 | 5.55632000  | #Ti |
| 6.52238000 | 10.61096000 | 2.36468000  | #Ti |
| 8.00260000 | 7.36006000  | 1.97399000  | #Ti |
| 0.60450000 | 10.61141000 | 15.15363000 | #Ti |
| 2.07445000 | 7.37450000  | 15.53066000 | #Ti |
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| 2.08522000 | 7.36013000  | 1.97553000  | #Ti |
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| 3.55777000 | 7.32826000  | 5.33541000 | #Ti |
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| 3.56370000 | 10.61177000 | 2.36470000 | #Ti |
| 5.04361000 | 7.36065000  | 1.97346000 | #Ti |

Rut-Glu-Z

1.000000000

|           |           |           |
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| 11.834800 | 0.000000  | 0.000000  |
| 0.000000  | 12.992946 | 0.000000  |
| 0.000000  | 0.000000  | 30.000000 |

H C N O Ti

9 5 1 164 80

Cartesian

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| 6.68208000 | 1.38092000 | 18.26281000 | #H |
| 8.87777000 | 5.01970000 | 19.81886000 | #H |
| 8.93796000 | 6.86861000 | 18.11047000 | #H |
| 7.30477000 | 6.95060000 | 18.08177000 | #H |
| 8.12551000 | 7.33951000 | 19.55864000 | #H |
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| 6.45694000 | 3.66532000 | 20.57274000 | #C |
| 5.97709000 | 2.71412000 | 19.48225000 | #C |
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| 7.98535000 | 5.26044000 | 19.22377000 | #C |
| 8.10385000 | 6.69147000 | 18.76639000 | #N |
| 4.86133000 | 2.76916000 | 18.98917000 | #O |
| 6.94715000 | 1.85393000 | 19.11056000 | #O |
| 9.20740000 | 4.23754000 | 17.42735000 | #O |
| 6.93941000 | 4.25540000 | 17.33943000 | #O |
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| 5.15489000 | 5.98284000 | 5.45755000  | #O |
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| 3.67327000 | 0.76961000 | 3.49068000  | #O |
| 5.15421000 | 5.24440000 | 2.03712000  | #O |
| 5.15261000 | 2.80352000 | 2.05495000  | #O |
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| 6.62927000 | 0.81018000 | 16.64318000 | #O |



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Rut-Glu-C

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H C N O Ti  
9 5 1 164 80

Cartesian

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H C N O Ti

9 5 1 164 80

Cartesian

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| 11.18649000 | 7.27204000  | 15.53001000 | #Ti |
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#### Rut-Gln-D

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0.000000 12.992946 0.000000

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H C N O Ti

10 5 2 163 80

Cartesian

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Rut-Gln-Z

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H C N O Ti

10 5 2 163 80

Cartesian

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H C N O Ti

14 6 4 162 80

Cartesian

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H C N O Ti

14 6 4 162 80

Cartesian

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H C N O Ti

14 6 4 162 80

Cartesian

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H C N O Ti

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H C N O Ti

14 6 2 162 80

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| 2.05066000 | 7.27888000  | 8.73055000  | #Ti |
| 0.68516000 | 7.30116000  | 5.32796000  | #Ti |
| 2.16512000 | 10.55344000 | 5.55149000  | #Ti |
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Rut-Lys-C

1.000000000

11.834800 0.000000 0.000000

0.000000 12.992946 0.000000

0.000000 0.000000 30.000000

H C N O Ti

14 6 2 162 80

Cartesian

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| 4.41458000 | 4.75174000  | 19.16278000 | #H |
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| 7.06353000 | 6.06482000  | 18.34384000 | #H |
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| 2.39437000 | 2.79603000 | 8.76668000  | #O |
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| 2.39266000 | 9.33196000  | 2.04429000  | #O |
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| 8.31646000 | 9.33378000  | 15.49852000 | #O |
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Rut-His-D

1.000000000

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0.000000 12.992946 0.000000

0.000000 0.000000 30.000000

H C N O Ti

9 6 3 162 80

Cartesian

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| 6.78878000 | 6.97783000 | 17.57388000 | #H |
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H C N O Ti

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Cartesian

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H C N O Ti

9 6 3 162 80

Cartesian

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*Amino acids adsorbed on anatase*

Ana-Phe-Z

1.000000000

15.138000 0.000000 0.000000

0.000000 20.478700 0.000000

0.000000 0.000000 30.000000

H C N O Ti

11 9 1 194 96

Cartesian

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Ana-Gly-D

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H C N O Ti

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Ana-Met-Z

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H C N O S Ti

11 5 1 98 1 48

Cartesian

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Ana-Glu-D

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H C N O Ti

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Ana-Cys-Z

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H C N O S Ti

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| 14.09474155 | 16.20133811 | 28.64213507 | #Ti |
| 10.30638136 | 5.96683747  | 28.59482507 | #Ti |
| 2.73651849  | 5.96321274  | 28.59590507 | #Ti |
| 10.30392900 | 16.20100840 | 28.64564507 | #Ti |
| 2.74694858  | 16.19862878 | 28.65290507 | #Ti |
| 8.41411471  | 11.08090130 | 28.63841507 | #Ti |
| 0.84800758  | 11.08751592 | 28.60991507 | #Ti |
| 8.41432513  | 0.84144891  | 28.61297507 | #Ti |
| 0.84912779  | 0.84271859  | 28.61069507 | #Ti |
| 4.63075157  | 11.07690796 | 28.66280507 | #Ti |
| 12.19885843 | 11.08966619 | 28.60463507 | #Ti |
| 4.63400624  | 0.84085503  | 28.61537507 | #Ti |
| 12.20002406 | 0.84415210  | 28.61213507 | #Ti |
| 8.41847445  | 3.60500852  | 28.06481507 | #Ti |
| 0.84396573  | 3.60664681  | 28.06526507 | #Ti |
| 8.41048462  | 13.85046117 | 28.08044507 | #Ti |
| 0.85248843  | 13.85855026 | 28.07639507 | #Ti |
| 4.62720928  | 3.60404602  | 28.06481507 | #Ti |
| 12.19950936 | 3.60824415  | 28.06643507 | #Ti |
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| 12.19838915 | 13.86080291 | 28.07273507 | #Ti |
| 6.51883862  | 8.73926435  | 28.05893507 | #Ti |
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| 14.09365161 | 18.96628618 | 28.09775507 | #Ti |
| 10.30409552 | 8.73705265  | 28.06409507 | #Ti |
| 2.73931902  | 8.73510718  | 28.06793507 | #Ti |
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| 2.74186221  | 18.96069549 | 28.10555507 | #Ti |

Ana-Ser-Z

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0.000000 10.239350 0.000000

0.000000 0.000000 25.000000

H C N O Ti

7 3 1 51 24

Cartesian

4.02625000 5.70785000 6.23731000 #H

5.32188000 6.52921000 6.97280000 #H

4.61988000 5.29698000 7.87784000 #H

2.49634000 6.48626000 7.88043000 #H

4.82262000 8.23966000 8.87543000 #H

3.12341000 8.29617000 9.44431000 #H

4.53485000 6.88816000 10.77905000 #H

3.27827000 8.08625000 6.62861000 #C

3.43852000 7.02994000 7.74166000 #C

3.91560000 7.63414000 9.05426000 #C

4.43914000 6.05030000 7.20719000 #N

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1.32613000 0.57052000 5.07564000 #O

3.26900000 5.63489000 4.94949000 #O

6.94308000 5.63664000 5.03413000 #O

5.08645000 3.53882000 4.35437000 #O

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| 3.20785000 | 8.72748000  | 3.87772000  | #O  |
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| 3.19933000 | 2.06863000  | 3.54751000  | #O  |
| 6.99330000 | 2.09631000  | 3.57742000  | #O  |
| 5.10760000 | 7.18134000  | 3.54899000  | #O  |
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Ana-Gln-D

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H C N O Ti

10 5 2 99 48

Cartesian

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| 6.31734747 | 5.15400487  | 8.30967321  | #H |
| 4.98458747 | 6.21370487  | 9.92184321  | #H |
| 4.10390747 | 3.38845487  | 7.33105321  | #H |
| 4.24615747 | 8.15994487  | 7.65481321  | #H |
| 3.38049747 | 7.98848487  | 9.15924321  | #H |
| 5.22265747 | 9.01869487  | 10.42420321 | #H |
| 6.35055747 | 8.79684487  | 9.07837321  | #H |
| 5.43432747 | 12.36134487 | 8.99502321  | #H |
| 6.06881747 | 11.33174487 | 10.26006321 | #H |
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| 4.83985747 | 6.47178487  | 8.85476321  | #C |
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| 5.01459747 | 10.38042487 | 8.75690321  | #C |
| 6.06660747 | 6.12393487  | 8.09170321  | #N |
| 5.53036747 | 11.43740487 | 9.40997321  | #N |
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| 2.47275747 | 18.37243487 | 6.42517321  | #O |
| 4.30081747 | 3.01212487  | 6.39711321  | #O |
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| 0.56821747 | 3.01299487  | 6.39132321  | #O |
| 0.56698747 | 13.23300487 | 6.47835321  | #O |
| 6.24523747 | 0.89283487  | 5.75899321  | #O |
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| 2.43867747 | 11.12465487 | 5.80219321  | #O |
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| 4.36772747 | 16.24919487 | 5.82873321  | #O |
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#### Ana-Lys-D

1.000000000

7.569000 0.000000 0.000000

0.000000 20.478700 0.000000

0.000000 0.000000 30.000000

H C N O Ti

14 6 2 98 48

Cartesian

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*Glycine adsorbed on the 9-layer (110) rutile surface*

Gly-D1-9layer

1.000000000

8.876100 0.000000 0.000000

0.000000 12.992946 0.000000

0.000000 0.000000 50.000000

H C N O Ti

5 2 1 218 108

Cartesian

5.40304000 5.11734000 32.36588000 #H

3.60839000 5.24393000 32.38221000 #H

5.59732000 7.27160000 30.20615000 #H

3.81579000 7.27318000 31.09599000 #H

4.91182000 7.43022000 32.33831000 #H

4.47571000 4.74186000 30.46723000 #C

4.52220000 5.46029000 31.80964000 #C

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| 7.39757000 | 3.06900000  | 14.80913000 | #O  |
| 5.91968000 | 1.08379000  | 13.50992000 | #O  |
| 5.91882000 | 10.82312000 | 12.80716000 | #O  |
| 7.39785000 | 2.36701000  | 11.52792000 | #O  |
| 7.39783000 | 12.79010000 | 11.52536000 | #O  |
| 5.91772000 | 4.33361000  | 10.26646000 | #O  |
| 5.91923000 | 1.08147000  | 9.53471000  | #O  |
| 7.39671000 | 12.08604000 | 8.23941000  | #O  |
| 7.39724000 | 3.07222000  | 8.24867000  | #O  |
| 5.91745000 | 1.08405000  | 6.95417000  | #O  |
| 5.91831000 | 10.82171000 | 6.24697000  | #O  |
| 7.39748000 | 2.37281000  | 4.93309000  | #O  |
| 7.39739000 | 12.78341000 | 4.93159000  | #O  |
| 5.91817000 | 10.82897000 | 3.66672000  | #O  |
| 5.91803000 | 1.08026000  | 2.91955000  | #O  |
| 7.39737000 | 12.05041000 | 1.50821000  | #O  |
| 7.39712000 | 3.10727000  | 1.51470000  | #O  |
| 5.91819000 | 1.08302000  | 0.33395000  | #O  |
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| 7.42784000 | 5.60469000  | 27.98917000 | #O  |
| 7.40080000 | 9.62453000  | 28.11003000 | #O  |
| 5.94295000 | 7.68466000  | 26.64862000 | #O  |
| 5.92249000 | 10.83383000 | 25.91636000 | #O  |
| 7.40718000 | 8.88715000  | 24.62782000 | #O  |
| 7.40352000 | 6.31483000  | 24.66179000 | #O  |
| 5.92080000 | 10.84070000 | 23.33481000 | #O  |
| 5.90968000 | 7.58188000  | 22.64753000 | #O  |
| 7.39773000 | 5.59855000  | 21.35671000 | #O  |
| 7.39933000 | 9.56509000  | 21.34937000 | #O  |
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| 5.91923000 | 10.82196000 | 19.33824000 | #O  |
| 7.39938000 | 8.85985000  | 18.07409000 | #O  |
| 7.39805000 | 6.29980000  | 18.08345000 | #O  |
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| 5.91666000 | 7.58109000  | 16.08770000 | #O  |
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| 7.39728000 | 9.55943000  | 14.79328000 | #O  |
| 5.91995000 | 7.57562000  | 13.51437000 | #O  |
| 5.91875000 | 4.33559000  | 12.82616000 | #O  |
| 7.39778000 | 8.86090000  | 11.52173000 | #O  |
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| 7.39755000 | 6.28958000  | 4.92219000  | #O  |
| 5.91985000 | 4.32924000  | 3.67471000  | #O  |
| 5.91963000 | 7.58072000  | 2.90166000  | #O  |
| 7.39752000 | 5.55543000  | 1.51015000  | #O  |
| 7.39756000 | 9.60179000  | 1.50298000  | #O  |
| 5.91741000 | 7.57624000  | 0.31598000  | #O  |
| 2.96858000 | 4.32812000  | 27.89942000 | #Ti |

|            |             |             |     |
|------------|-------------|-------------|-----|
| 4.44450000 | 1.08870000  | 28.15268000 | #Ti |
| 2.96479000 | 1.08225000  | 24.83238000 | #Ti |
| 4.44049000 | 4.33268000  | 24.71896000 | #Ti |
| 2.96645000 | 4.32933000  | 21.33515000 | #Ti |
| 4.43994000 | 1.07775000  | 21.43190000 | #Ti |
| 2.96102000 | 1.08418000  | 18.13183000 | #Ti |
| 4.43894000 | 4.33379000  | 18.10025000 | #Ti |
| 2.95899000 | 10.82406000 | 14.80366000 | #Ti |
| 4.43690000 | 1.08259000  | 14.80111000 | #Ti |
| 2.95950000 | 1.08403000  | 11.47116000 | #Ti |
| 4.43817000 | 10.82728000 | 11.57091000 | #Ti |
| 2.95913000 | 10.82665000 | 8.35453000  | #Ti |
| 4.44006000 | 1.08437000  | 8.16646000  | #Ti |
| 2.95923000 | 1.08280000  | 4.76024000  | #Ti |
| 4.43844000 | 10.82717000 | 5.08145000  | #Ti |
| 2.95909000 | 10.82629000 | 1.86286000  | #Ti |
| 4.43857000 | 1.08315000  | 1.41615000  | #Ti |
| 0.00928000 | 4.36013000  | 27.66884000 | #Ti |
| 1.48243000 | 1.10061000  | 28.17440000 | #Ti |
| 8.87458000 | 1.09550000  | 24.83285000 | #Ti |
| 1.52169000 | 4.31814000  | 24.51918000 | #Ti |
| 0.00052000 | 4.33204000  | 21.30273000 | #Ti |
| 1.47969000 | 1.08430000  | 21.42870000 | #Ti |
| 0.00562000 | 1.08457000  | 18.12610000 | #Ti |
| 1.48523000 | 4.33306000  | 18.08207000 | #Ti |
| 0.00096000 | 10.82794000 | 14.80123000 | #Ti |
| 1.48157000 | 1.08394000  | 14.79853000 | #Ti |
| 0.00230000 | 1.08472000  | 11.47858000 | #Ti |
| 1.47981000 | 10.82838000 | 11.56965000 | #Ti |
| 0.00070000 | 10.82695000 | 8.35317000  | #Ti |
| 1.47878000 | 1.08442000  | 8.16707000  | #Ti |
| 0.00052000 | 1.08299000  | 4.76135000  | #Ti |
| 1.47966000 | 10.82680000 | 5.07982000  | #Ti |
| 0.00041000 | 10.82674000 | 1.86270000  | #Ti |
| 1.47934000 | 1.08339000  | 1.41587000  | #Ti |
| 0.00332000 | 10.85542000 | 27.72993000 | #Ti |
| 1.50705000 | 7.59647000  | 28.13707000 | #Ti |
| 0.01310000 | 7.58942000  | 24.81769000 | #Ti |
| 1.47937000 | 10.85122000 | 24.50808000 | #Ti |
| 8.87604000 | 10.82751000 | 21.24643000 | #Ti |
| 1.45865000 | 7.57587000  | 21.33041000 | #Ti |
| 8.87343000 | 7.57928000  | 18.10807000 | #Ti |
| 1.47982000 | 10.82867000 | 18.03336000 | #Ti |
| 0.00099000 | 4.32931000  | 14.85071000 | #Ti |
| 1.46209000 | 7.57537000  | 14.74144000 | #Ti |
| 8.87435000 | 7.57957000  | 11.44100000 | #Ti |
| 1.48064000 | 4.33225000  | 11.60141000 | #Ti |
| 0.00064000 | 4.33035000  | 8.38022000  | #Ti |
| 1.47682000 | 7.57654000  | 8.14032000  | #Ti |
| 0.00037000 | 7.57758000  | 4.73892000  | #Ti |
| 1.47952000 | 4.33072000  | 5.09382000  | #Ti |
| 0.00059000 | 4.33062000  | 1.87291000  | #Ti |
| 1.47928000 | 7.57702000  | 1.39739000  | #Ti |
| 2.96206000 | 10.84173000 | 27.72027000 | #Ti |
| 4.34573000 | 7.58348000  | 27.85889000 | #Ti |

|            |             |             |     |
|------------|-------------|-------------|-----|
| 2.95292000 | 7.58822000  | 24.57429000 | #Ti |
| 4.44065000 | 10.83725000 | 24.50272000 | #Ti |
| 2.95738000 | 10.82755000 | 21.24753000 | #Ti |
| 4.44518000 | 7.58343000  | 21.30235000 | #Ti |
| 2.95884000 | 7.58060000  | 17.99467000 | #Ti |
| 4.43873000 | 10.82827000 | 18.03161000 | #Ti |
| 2.96026000 | 4.33151000  | 14.85612000 | #Ti |
| 4.45364000 | 7.57661000  | 14.73249000 | #Ti |
| 2.95867000 | 7.57878000  | 11.42550000 | #Ti |
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| 2.95935000 | 4.33122000  | 8.37886000  | #Ti |
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| 4.43843000 | 4.33059000  | 5.09236000  | #Ti |
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| 4.43861000 | 7.57733000  | 1.39807000  | #Ti |
| 5.93178000 | 4.34098000  | 27.88501000 | #Ti |
| 7.40253000 | 1.10118000  | 28.17240000 | #Ti |
| 5.92396000 | 1.08469000  | 24.83027000 | #Ti |
| 7.36120000 | 4.33693000  | 24.50944000 | #Ti |
| 5.91376000 | 4.33330000  | 21.32941000 | #Ti |
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| 5.91572000 | 1.08432000  | 18.13115000 | #Ti |
| 7.39414000 | 4.32280000  | 18.07602000 | #Ti |
| 5.91872000 | 10.82683000 | 14.80125000 | #Ti |
| 7.39646000 | 1.08423000  | 14.80327000 | #Ti |
| 5.91648000 | 1.08441000  | 11.47900000 | #Ti |
| 7.39771000 | 10.83310000 | 11.56885000 | #Ti |
| 5.91792000 | 10.82684000 | 8.35452000  | #Ti |
| 7.39703000 | 1.08435000  | 8.17291000  | #Ti |
| 5.91817000 | 1.08272000  | 4.76050000  | #Ti |
| 7.39718000 | 10.82681000 | 5.08015000  | #Ti |
| 5.91794000 | 10.82634000 | 1.86294000  | #Ti |
| 7.39786000 | 1.08336000  | 1.41581000  | #Ti |
| 5.91978000 | 10.83114000 | 27.72005000 | #Ti |
| 7.45348000 | 7.59903000  | 28.14450000 | #Ti |
| 5.92685000 | 7.59535000  | 24.77772000 | #Ti |
| 7.40086000 | 10.83742000 | 24.50572000 | #Ti |
| 5.92093000 | 10.82730000 | 21.24496000 | #Ti |
| 7.39198000 | 7.57775000  | 21.49482000 | #Ti |
| 5.92235000 | 7.58068000  | 18.09130000 | #Ti |
| 7.39819000 | 10.83905000 | 18.02944000 | #Ti |
| 5.91716000 | 4.32951000  | 14.85316000 | #Ti |
| 7.40000000 | 7.57590000  | 14.82329000 | #Ti |
| 5.92115000 | 7.57919000  | 11.44112000 | #Ti |
| 7.39699000 | 4.32816000  | 11.60051000 | #Ti |
| 5.91788000 | 4.33106000  | 8.37904000  | #Ti |
| 7.39702000 | 7.57673000  | 8.15153000  | #Ti |
| 5.91828000 | 7.57843000  | 4.73783000  | #Ti |
| 7.39724000 | 4.33067000  | 5.09370000  | #Ti |
| 5.91818000 | 4.33106000  | 1.87275000  | #Ti |
| 7.39784000 | 7.57689000  | 1.39708000  | #Ti |

*Water adsorption on the (110) rutile surface*

H<sub>2</sub>O-4layer

1.000000000

5.953169 0.000000 0.000000

0.000000 13.020442 0.000000

0.000000 0.000000 30.000000

H O Ti

2 65 32

Cartesian

|            |             |             |    |
|------------|-------------|-------------|----|
| 0.83975000 | 8.71303000  | 18.67729000 | #H |
| 1.56243000 | 10.01853000 | 18.14337000 | #H |
| 4.48711000 | 11.76925000 | 17.43730000 | #O |
| 5.92437000 | 9.82139000  | 16.09708000 | #O |
| 0.02055000 | 0.80411000  | 16.27574000 | #O |
| 4.48051000 | 11.87508000 | 14.86939000 | #O |
| 4.47372000 | 2.00639000  | 14.09169000 | #O |
| 0.01177000 | 0.05503000  | 12.82452000 | #O |
| 0.00465000 | 10.50634000 | 12.87209000 | #O |
| 4.47248000 | 2.02320000  | 11.51011000 | #O |
| 4.47035000 | 11.76704000 | 10.83964000 | #O |
| 0.01051000 | 9.80188000  | 9.51322000  | #O |
| 0.00814000 | 0.71913000  | 9.50148000  | #O |
| 4.46738000 | 11.76075000 | 8.26063000  | #O |
| 4.47094000 | 8.54150000  | 7.48056000  | #O |
| 0.00455000 | 13.01968200 | 6.12182000  | #O |
| 0.00495000 | 10.55927000 | 6.08903000  | #O |
| 4.47529000 | 8.52358000  | 4.90292000  | #O |
| 1.51250000 | 11.67400000 | 17.45449000 | #O |
| 3.03524000 | 9.81962000  | 16.09338000 | #O |
| 2.98434000 | 0.80522000  | 16.27913000 | #O |
| 1.50618000 | 11.86933000 | 14.87432000 | #O |
| 1.49548000 | 2.00843000  | 14.08777000 | #O |
| 2.98400000 | 0.05478000  | 12.82304000 | #O |
| 2.98660000 | 10.50529000 | 12.87747000 | #O |
| 1.49734000 | 2.02381000  | 11.50872000 | #O |
| 1.49448000 | 11.76711000 | 10.83918000 | #O |
| 2.98447000 | 9.80295000  | 9.51017000  | #O |
| 2.98465000 | 0.71890000  | 9.49993000  | #O |
| 1.48944000 | 11.76160000 | 8.26031000  | #O |
| 1.49578000 | 8.53949000  | 7.47657000  | #O |
| 2.98117000 | 13.01947200 | 6.12249000  | #O |
| 2.98094000 | 10.55961000 | 6.08895000  | #O |
| 1.49860000 | 8.52341000  | 4.90293000  | #O |
| 4.48499000 | 5.27768000  | 17.46596000 | #O |
| 0.00994000 | 3.26583000  | 16.22914000 | #O |
| 0.01304000 | 7.32933000  | 16.28035000 | #O |
| 4.49323000 | 5.29264000  | 14.89140000 | #O |
| 4.48252000 | 8.48635000  | 14.05607000 | #O |
| 0.01435000 | 6.54742000  | 12.83852000 | #O |
| 0.00899000 | 3.98569000  | 12.85961000 | #O |
| 4.47393000 | 8.53090000  | 11.51838000 | #O |
| 4.46921000 | 5.25387000  | 10.83932000 | #O |
| 0.00955000 | 3.28962000  | 9.50265000  | #O |
| 0.00754000 | 7.22924000  | 9.50530000  | #O |

|            |             |             |     |
|------------|-------------|-------------|-----|
| 4.46846000 | 5.25193000  | 8.26046000  | #O  |
| 4.47567000 | 2.02287000  | 7.46508000  | #O  |
| 0.00426000 | 6.50978000  | 6.12689000  | #O  |
| 0.00486000 | 4.04737000  | 6.08854000  | #O  |
| 4.47659000 | 2.01128000  | 4.89041000  | #O  |
| 1.51011000 | 5.28683000  | 17.46610000 | #O  |
| 2.99024000 | 3.26740000  | 16.22294000 | #O  |
| 3.00749000 | 7.31477000  | 16.23225000 | #O  |
| 1.50170000 | 5.28292000  | 14.89662000 | #O  |
| 1.49448000 | 8.51248000  | 14.10764000 | #O  |
| 2.98292000 | 6.54929000  | 12.84679000 | #O  |
| 2.98792000 | 3.98670000  | 12.86504000 | #O  |
| 1.50304000 | 8.52793000  | 11.51239000 | #O  |
| 1.49468000 | 5.25543000  | 10.83872000 | #O  |
| 2.98684000 | 3.28920000  | 9.50227000  | #O  |
| 2.98407000 | 7.22895000  | 9.50273000  | #O  |
| 1.49072000 | 5.25185000  | 8.26054000  | #O  |
| 1.49896000 | 2.02377000  | 7.46478000  | #O  |
| 2.98060000 | 6.50978000  | 6.12713000  | #O  |
| 2.98179000 | 4.04741000  | 6.08879000  | #O  |
| 1.50018000 | 2.01070000  | 4.89018000  | #O  |
| 1.60203000 | 9.01841000  | 18.15934000 | #O  |
| 4.47697000 | 2.03572000  | 15.88167000 | #Ti |
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| 4.47558000 | 11.81029000 | 13.04705000 | #Ti |
| 0.00868000 | 2.04076000  | 12.64498000 | #Ti |
| 4.47469000 | 8.52506000  | 9.29921000  | #Ti |
| 0.00712000 | 11.77703000 | 9.69873000  | #Ti |
| 4.46875000 | 11.78450000 | 6.46673000  | #Ti |
| 0.01168000 | 8.53422000  | 5.97392000  | #Ti |
| 1.49816000 | 2.04021000  | 15.87846000 | #Ti |
| 3.01256000 | 11.81545000 | 16.34748000 | #Ti |
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| 2.98437000 | 2.04056000  | 12.64624000 | #Ti |
| 1.49853000 | 8.52339000  | 9.29076000  | #Ti |
| 2.98214000 | 11.77714000 | 9.69760000  | #Ti |
| 1.49206000 | 11.78601000 | 6.46585000  | #Ti |
| 2.98919000 | 8.53424000  | 5.97395000  | #Ti |
| 4.48326000 | 8.56505000  | 15.83760000 | #Ti |
| 0.01958000 | 5.30183000  | 16.39166000 | #Ti |
| 4.47816000 | 5.29218000  | 13.07293000 | #Ti |
| 0.02262000 | 8.54624000  | 12.66402000 | #Ti |
| 4.47390000 | 2.01387000  | 9.27887000  | #Ti |
| 0.00686000 | 5.26873000  | 9.70265000  | #Ti |
| 4.46891000 | 5.27536000  | 6.46832000  | #Ti |
| 0.01144000 | 2.02428000  | 5.96141000  | #Ti |
| 1.51636000 | 8.53844000  | 15.96128000 | #Ti |
| 2.99760000 | 5.30115000  | 16.38995000 | #Ti |
| 1.50049000 | 5.28936000  | 13.07821000 | #Ti |
| 2.97728000 | 8.54545000  | 12.66967000 | #Ti |
| 1.49737000 | 2.01431000  | 9.27870000  | #Ti |
| 2.98304000 | 5.26870000  | 9.70101000  | #Ti |
| 1.49219000 | 5.27553000  | 6.46823000  | #Ti |
| 2.98800000 | 2.02432000  | 5.96145000  | #Ti |

H<sub>2</sub>O-5layer

1.00000000

|          |           |           |
|----------|-----------|-----------|
| 5.953169 | 0.000000  | 0.000000  |
| 0.000000 | 13.020442 | 0.000000  |
| 0.000000 | 0.000000  | 30.000000 |

H O Ti

2 81 40

Cartesian

|            |             |             |    |
|------------|-------------|-------------|----|
| 0.84857000 | 8.75392000  | 18.68143000 | #H |
| 1.54876000 | 10.06276000 | 18.08508000 | #H |
| 4.49425000 | 11.74962000 | 17.32864000 | #O |
| 5.92800900 | 9.79116000  | 16.05261000 | #O |
| 0.03272000 | 0.79496000  | 16.26776000 | #O |
| 4.48843000 | 11.86215000 | 14.76928000 | #O |
| 4.48732000 | 1.98744000  | 14.09276000 | #O |
| 0.02518000 | 0.06067000  | 12.78077000 | #O |
| 0.02037000 | 10.47799000 | 12.82922000 | #O |
| 4.48259000 | 2.01324000  | 11.52443000 | #O |
| 4.49145000 | 11.76301000 | 10.82521000 | #O |
| 0.01832000 | 9.76987000  | 9.52943000  | #O |
| 0.01757000 | 0.74285000  | 9.53112000  | #O |
| 4.48899000 | 11.77054000 | 8.22650000  | #O |
| 4.48288000 | 8.52491000  | 7.54087000  | #O |
| 0.02019000 | 0.06116000  | 6.23923000  | #O |
| 0.02198000 | 10.47859000 | 6.24227000  | #O |
| 4.48195000 | 8.51912000  | 4.98065000  | #O |
| 4.48355000 | 11.78717000 | 4.26269000  | #O |
| 0.01585000 | 9.75227000  | 2.84422000  | #O |
| 0.01636000 | 0.79443000  | 2.82875000  | #O |
| 4.47987000 | 11.78346000 | 1.69267000  | #O |
| 1.51670000 | 11.64060000 | 17.34505000 | #O |
| 3.04541000 | 9.78608000  | 16.05818000 | #O |
| 2.98971000 | 0.79649000  | 16.27332000 | #O |
| 1.51480000 | 11.85656000 | 14.77472000 | #O |
| 1.50844000 | 1.99356000  | 14.08940000 | #O |
| 2.99870000 | 0.06098000  | 12.78123000 | #O |
| 3.00342000 | 10.47678000 | 12.83193000 | #O |
| 1.50825000 | 2.01577000  | 11.52401000 | #O |
| 1.51726000 | 11.75903000 | 10.82675000 | #O |
| 2.99168000 | 9.77107000  | 9.52698000  | #O |
| 2.99340000 | 0.74274000  | 9.53010000  | #O |
| 1.50759000 | 11.77428000 | 8.23014000  | #O |
| 1.50453000 | 8.52308000  | 7.53979000  | #O |
| 2.99665000 | 0.06081000  | 6.24031000  | #O |
| 2.99646000 | 10.47913000 | 6.24374000  | #O |
| 1.50701000 | 8.51888000  | 4.98025000  | #O |
| 1.50727000 | 11.78760000 | 4.26295000  | #O |
| 2.99298000 | 9.75230000  | 2.84275000  | #O |
| 2.99279000 | 0.79414000  | 2.82914000  | #O |
| 1.50340000 | 11.78360000 | 1.69276000  | #O |
| 4.48711000 | 5.27109000  | 17.35472000 | #O |
| 0.01702000 | 3.23907000  | 16.21814000 | #O |
| 0.02401000 | 7.32367000  | 16.27119000 | #O |
| 4.49332000 | 5.28545000  | 14.78912000 | #O |
| 4.49047000 | 8.45615000  | 14.04696000 | #O |

|            |             |             |     |
|------------|-------------|-------------|-----|
| 0.02704000 | 6.55450000  | 12.79428000 | #O  |
| 0.02079000 | 3.95529000  | 12.81915000 | #O  |
| 4.48122000 | 8.52279000  | 11.52742000 | #O  |
| 4.49012000 | 5.24924000  | 10.82759000 | #O  |
| 0.01592000 | 3.25720000  | 9.52645000  | #O  |
| 0.01797000 | 7.25323000  | 9.53029000  | #O  |
| 4.49208000 | 5.25534000  | 8.22768000  | #O  |
| 4.48201000 | 2.00840000  | 7.53409000  | #O  |
| 0.02138000 | 6.57099000  | 6.24525000  | #O  |
| 0.02161000 | 3.96414000  | 6.24252000  | #O  |
| 4.48113000 | 2.00826000  | 4.97299000  | #O  |
| 4.48401000 | 5.27317000  | 4.27004000  | #O  |
| 0.01672000 | 3.23934000  | 2.83824000  | #O  |
| 0.01585000 | 7.30637000  | 2.83767000  | #O  |
| 4.48045000 | 5.27253000  | 1.70042000  | #O  |
| 1.51363000 | 5.27340000  | 17.35182000 | #O  |
| 3.00349000 | 3.23915000  | 16.21026000 | #O  |
| 3.00276000 | 7.30675000  | 16.21021000 | #O  |
| 1.50525000 | 5.27555000  | 14.78758000 | #O  |
| 1.50568000 | 8.49529000  | 14.09531000 | #O  |
| 2.99791000 | 6.55466000  | 12.80019000 | #O  |
| 3.00234000 | 3.95631000  | 12.82218000 | #O  |
| 1.51058000 | 8.51956000  | 11.52356000 | #O  |
| 1.51545000 | 5.24638000  | 10.82649000 | #O  |
| 2.99330000 | 3.25651000  | 9.52508000  | #O  |
| 2.99208000 | 7.25473000  | 9.52910000  | #O  |
| 1.51370000 | 5.25559000  | 8.22753000  | #O  |
| 1.50497000 | 2.00879000  | 7.53432000  | #O  |
| 2.99794000 | 6.57096000  | 6.24677000  | #O  |
| 2.99839000 | 3.96426000  | 6.24378000  | #O  |
| 1.50507000 | 2.00875000  | 4.97311000  | #O  |
| 1.50832000 | 5.27313000  | 4.26991000  | #O  |
| 2.99315000 | 3.23920000  | 2.83742000  | #O  |
| 2.99375000 | 7.30604000  | 2.83731000  | #O  |
| 1.50366000 | 5.27277000  | 1.70023000  | #O  |
| 1.59640000 | 9.05741000  | 18.13757000 | #O  |
| 4.48896000 | 2.00545000  | 15.90094000 | #Ti |
| 0.02016000 | 11.78311000 | 16.22258000 | #Ti |
| 4.48268000 | 11.84512000 | 12.87898000 | #Ti |
| 0.01419000 | 2.08579000  | 12.71227000 | #Ti |
| 4.40272000 | 8.51610000  | 9.57378000  | #Ti |
| 5.82361000 | 11.76434000 | 9.50746000  | #Ti |
| 4.47890000 | 11.84400000 | 6.12072000  | #Ti |
| 0.00860000 | 8.60003000  | 6.35556000  | #Ti |
| 4.48155000 | 8.52575000  | 3.17151000  | #Ti |
| 0.01274000 | 11.78017000 | 2.77095000  | #Ti |
| 1.50954000 | 2.02197000  | 15.89768000 | #Ti |
| 3.02141000 | 11.79244000 | 16.22756000 | #Ti |
| 1.50545000 | 11.84505000 | 12.90218000 | #Ti |
| 2.99093000 | 2.08453000  | 12.71475000 | #Ti |
| 1.42668000 | 8.50418000  | 9.53554000  | #Ti |
| 2.84228000 | 11.76420000 | 9.52324000  | #Ti |
| 1.50326000 | 11.84138000 | 6.12011000  | #Ti |
| 2.99367000 | 8.59874000  | 6.35984000  | #Ti |
| 1.50529000 | 8.52547000  | 3.17449000  | #Ti |



|            |             |             |     |
|------------|-------------|-------------|-----|
| 2.98975000 | 11.78009000 | 2.77098000  | #Ti |
| 4.49340000 | 8.54926000  | 15.84434000 | #Ti |
| 0.02298000 | 5.27744000  | 16.27125000 | #Ti |
| 4.48467000 | 5.33383000  | 12.91555000 | #Ti |
| 0.03302000 | 8.59429000  | 12.73493000 | #Ti |
| 4.39582000 | 1.99892000  | 9.52871000  | #Ti |
| 5.81802000 | 5.25728000  | 9.52636000  | #Ti |
| 4.48048000 | 5.33308000  | 6.13142000  | #Ti |
| 0.01246000 | 2.08827000  | 6.34309000  | #Ti |
| 4.48200000 | 2.01487000  | 3.16344000  | #Ti |
| 0.01336000 | 5.27165000  | 2.77920000  | #Ti |
| 1.52589000 | 8.50591000  | 15.99770000 | #Ti |
| 3.00357000 | 5.27298000  | 16.26996000 | #Ti |
| 1.50786000 | 5.32646000  | 12.91952000 | #Ti |
| 2.96895000 | 8.59367000  | 12.75023000 | #Ti |
| 1.41959000 | 2.00255000  | 9.52870000  | #Ti |
| 2.84124000 | 5.25854000  | 9.52636000  | #Ti |
| 1.50313000 | 5.33448000  | 6.13187000  | #Ti |
| 2.98888000 | 2.08931000  | 6.34344000  | #Ti |
| 1.50536000 | 2.01433000  | 3.16320000  | #Ti |
| 2.98991000 | 5.27169000  | 2.77929000  | #Ti |

H<sub>2</sub>O-6layer

1.000000000

|          |           |           |
|----------|-----------|-----------|
| 5.953169 | 0.000000  | 0.000000  |
| 0.000000 | 13.020442 | 0.000000  |
| 0.000000 | 0.000000  | 35.000000 |

H O Ti

2 97 48

Cartesian

|            |            |             |    |
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| 2.98435000 | 6.32694000 | 20.20386000 | #H |
| 2.24936000 | 5.00950000 | 20.69593000 | #H |
| 5.95223900 | 1.62291000 | 19.46054000 | #O |
| 1.43594000 | 6.15033000 | 18.13317000 | #O |
| 1.47935000 | 3.66225000 | 18.29504000 | #O |
| 0.00248000 | 1.62970000 | 16.89281000 | #O |
| 0.00041000 | 4.84735000 | 16.08214000 | #O |
| 1.48993000 | 2.90560000 | 14.86621000 | #O |
| 1.48625000 | 0.33220000 | 14.87663000 | #O |
| 5.95234900 | 4.88437000 | 13.54877000 | #O |
| 5.95271900 | 1.62347000 | 12.87391000 | #O |
| 1.48864000 | 6.15481000 | 11.55518000 | #O |
| 1.48906000 | 3.60571000 | 11.55640000 | #O |
| 5.95248900 | 1.62596000 | 10.31092000 | #O |
| 5.95294900 | 4.88231000 | 9.54257000  | #O |
| 1.48747000 | 2.89836000 | 8.28643000  | #O |
| 1.48664000 | 0.35479000 | 8.28628000  | #O |
| 5.95288900 | 4.88253000 | 6.97857000  | #O |
| 5.95294900 | 1.62537000 | 6.29735000  | #O |
| 1.48813000 | 6.17235000 | 4.97817000  | #O |
| 1.48843000 | 3.59453000 | 4.97634000  | #O |
| 5.95315900 | 1.62860000 | 3.72340000  | #O |
| 0.00012000 | 4.88687000 | 2.95447000  | #O |
| 1.48864000 | 2.86364000 | 1.57406000  | #O |

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|------------|-------------|-------------|----|
| 1.48923000 | 0.40346000  | 1.57182000  | #O |
| 5.95314900 | 4.88451000  | 0.37465000  | #O |
| 0.00013000 | 8.12000000  | 19.45489000 | #O |
| 1.48548000 | 12.61678000 | 18.25904000 | #O |
| 1.49963000 | 10.15712000 | 18.29928000 | #O |
| 5.94713900 | 8.18695000  | 16.88716000 | #O |
| 0.00043000 | 11.38073000 | 16.12541000 | #O |
| 1.48878000 | 9.43130000  | 14.86484000 | #O |
| 1.48738000 | 6.85559000  | 14.88285000 | #O |
| 5.95304900 | 11.39531000 | 13.54531000 | #O |
| 5.95254900 | 8.13723000  | 12.87432000 | #O |
| 1.48793000 | 12.66270000 | 11.55292000 | #O |
| 1.48806000 | 10.11727000 | 11.55339000 | #O |
| 5.95299900 | 8.13765000  | 10.31101000 | #O |
| 5.95296900 | 11.39057000 | 9.53294000  | #O |
| 1.48686000 | 9.40925000  | 8.28615000  | #O |
| 1.48768000 | 6.86657000  | 8.28661000  | #O |
| 5.95251900 | 11.39243000 | 6.97414000  | #O |
| 5.95276900 | 8.13986000  | 6.29761000  | #O |
| 1.48821000 | 12.68052000 | 4.97197000  | #O |
| 1.48791000 | 10.10481000 | 4.96913000  | #O |
| 0.00002000 | 8.13714000  | 3.72325000  | #O |
| 5.95275900 | 11.40028000 | 2.94652000  | #O |
| 1.48906000 | 9.37411000  | 1.57371000  | #O |
| 1.48932000 | 6.91395000  | 1.57261000  | #O |
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| 2.97658000 | 1.62751000  | 19.45856000 | #O |
| 4.50103000 | 6.14272000  | 18.14545000 | #O |
| 4.46898000 | 3.65008000  | 18.24154000 | #O |
| 2.97172000 | 1.62441000  | 16.89408000 | #O |
| 2.97085000 | 4.87211000  | 16.13485000 | #O |
| 4.46150000 | 2.90650000  | 14.87027000 | #O |
| 4.46586000 | 0.33388000  | 14.87752000 | #O |
| 2.97676000 | 4.88295000  | 13.54210000 | #O |
| 2.97601000 | 1.62075000  | 12.87399000 | #O |
| 4.46403000 | 6.15496000  | 11.55480000 | #O |
| 4.46392000 | 3.60541000  | 11.55687000 | #O |
| 2.97620000 | 1.62674000  | 10.31060000 | #O |
| 2.97647000 | 4.88164000  | 9.53876000  | #O |
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| 2.97652000 | 4.88254000  | 6.97895000  | #O |
| 2.97638000 | 1.62519000  | 6.29719000  | #O |
| 4.46494000 | 6.17234000  | 4.97801000  | #O |
| 4.46470000 | 3.59461000  | 4.97707000  | #O |
| 2.97672000 | 1.62852000  | 3.72340000  | #O |
| 2.97729000 | 4.88767000  | 2.95454000  | #O |
| 4.46546000 | 2.86360000  | 1.57428000  | #O |
| 4.46581000 | 0.40341000  | 1.57187000  | #O |
| 2.97658000 | 4.88475000  | 0.37435000  | #O |
| 2.97439000 | 8.01035000  | 19.47796000 | #O |
| 4.47144000 | 12.61685000 | 18.25655000 | #O |
| 4.45636000 | 10.15736000 | 18.30331000 | #O |
| 2.97575000 | 8.18393000  | 16.89365000 | #O |
| 2.97799000 | 11.38288000 | 16.12170000 | #O |

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|------------|-------------|-------------|-----|
| 4.46290000 | 9.43138000  | 14.86455000 | #O  |
| 4.46504000 | 6.85537000  | 14.88439000 | #O  |
| 2.97663000 | 11.39566000 | 13.54400000 | #O  |
| 2.97623000 | 8.13676000  | 12.87381000 | #O  |
| 4.46495000 | 12.66259000 | 11.55287000 | #O  |
| 4.46461000 | 10.11726000 | 11.55292000 | #O  |
| 2.97655000 | 8.13751000  | 10.31094000 | #O  |
| 2.97659000 | 11.39150000 | 9.53214000  | #O  |
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| 4.46397000 | 6.86657000  | 8.28654000  | #O  |
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| 2.97616000 | 8.13977000  | 6.29740000  | #O  |
| 4.46497000 | 12.68060000 | 4.97189000  | #O  |
| 4.46472000 | 10.10488000 | 4.96913000  | #O  |
| 2.97653000 | 8.13687000  | 3.72329000  | #O  |
| 2.97633000 | 11.40053000 | 2.94642000  | #O  |
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| 4.46605000 | 6.91352000  | 1.57220000  | #O  |
| 2.97662000 | 11.39666000 | 0.36945000  | #O  |
| 3.02629000 | 5.32950000  | 20.20440000 | #O  |
| 0.00036000 | 4.89693000  | 17.86907000 | #Ti |
| 1.48673000 | 1.63371000  | 18.38414000 | #Ti |
| 5.95227900 | 1.63329000  | 15.06395000 | #Ti |
| 1.50225000 | 4.88580000  | 14.71277000 | #Ti |
| 5.95249900 | 4.88092000  | 11.40905000 | #Ti |
| 1.48781000 | 1.62612000  | 11.70359000 | #Ti |
| 5.95169900 | 1.62596000  | 8.45579000  | #Ti |
| 1.48638000 | 4.88065000  | 8.14939000  | #Ti |
| 5.95291900 | 4.88236000  | 4.77877000  | #Ti |
| 1.48797000 | 1.62607000  | 5.14878000  | #Ti |
| 0.00058000 | 1.63180000  | 1.92709000  | #Ti |
| 1.48844000 | 4.88614000  | 1.44900000  | #Ti |
| 0.00252000 | 11.38601000 | 17.91895000 | #Ti |
| 1.48152000 | 8.13651000  | 18.36100000 | #Ti |
| 5.95239900 | 8.14671000  | 15.05299000 | #Ti |
| 1.48823000 | 11.40038000 | 14.69325000 | #Ti |
| 5.95230900 | 11.39063000 | 11.38711000 | #Ti |
| 1.48813000 | 8.13550000  | 11.70085000 | #Ti |
| 5.95184900 | 8.13671000  | 8.45469000  | #Ti |
| 1.48701000 | 11.39143000 | 8.14031000  | #Ti |
| 5.95287900 | 11.39249000 | 4.77049000  | #Ti |
| 1.48783000 | 8.13643000  | 5.14874000  | #Ti |
| 0.00068000 | 8.14204000  | 1.92712000  | #Ti |
| 1.48886000 | 11.39707000 | 1.44330000  | #Ti |
| 2.98632000 | 4.87270000  | 17.99868000 | #Ti |
| 4.46616000 | 1.63261000  | 18.38403000 | #Ti |
| 2.97566000 | 1.63140000  | 15.06746000 | #Ti |
| 4.45355000 | 4.88587000  | 14.70978000 | #Ti |
| 2.97575000 | 4.87993000  | 11.39558000 | #Ti |
| 4.46379000 | 1.62633000  | 11.70346000 | #Ti |
| 2.97514000 | 1.62633000  | 8.45513000  | #Ti |
| 4.46580000 | 4.88064000  | 8.14936000  | #Ti |
| 2.97638000 | 4.88210000  | 4.77954000  | #Ti |
| 4.46469000 | 1.62612000  | 5.14878000  | #Ti |
| 2.97723000 | 1.63184000  | 1.92710000  | #Ti |

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|------------|-------------|-------------|-----|
| 4.46470000 | 4.88622000  | 1.44884000  | #Ti |
| 2.97753000 | 11.39624000 | 17.91584000 | #Ti |
| 4.47361000 | 8.14407000  | 18.36793000 | #Ti |
| 2.97559000 | 8.14508000  | 15.06366000 | #Ti |
| 4.46411000 | 11.39919000 | 14.69319000 | #Ti |
| 2.97578000 | 11.39122000 | 11.38687000 | #Ti |
| 4.46303000 | 8.13524000  | 11.70062000 | #Ti |
| 2.97523000 | 8.13615000  | 8.45335000  | #Ti |
| 4.46356000 | 11.39144000 | 8.14011000  | #Ti |
| 2.97630000 | 11.39249000 | 4.77047000  | #Ti |
| 4.46462000 | 8.13640000  | 5.14859000  | #Ti |
| 2.97727000 | 8.14195000  | 1.92733000  | #Ti |
| 4.46540000 | 11.39706000 | 1.44328000  | #Ti |

H<sub>2</sub>O-7layer

1.000000000

|          |           |           |
|----------|-----------|-----------|
| 5.953169 | 0.000000  | 0.000000  |
| 0.000000 | 13.020442 | 0.000000  |
| 0.000000 | 0.000000  | 35.000000 |

H O Ti

2 113 56

Cartesian

|            |             |             |    |
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| 5.74699000 | 8.36489000  | 24.17192000 | #H |
| 0.86915000 | 9.35582000  | 24.41179000 | #H |
| 0.00077000 | 0.00383000  | 22.85487000 | #O |
| 1.48752000 | 4.44338000  | 21.70941000 | #O |
| 1.48857000 | 2.06751000  | 21.70892000 | #O |
| 0.00029000 | 6.50855000  | 20.32007000 | #O |
| 5.95310900 | 3.25493000  | 19.75800000 | #O |
| 1.48832000 | 1.29304000  | 18.41384000 | #O |
| 1.48817000 | 5.21643000  | 18.41377000 | #O |
| 0.00000000 | 3.25507000  | 17.15733000 | #O |
| 0.00014000 | 0.00030000  | 16.43038000 | #O |
| 1.48811000 | 4.52629000  | 15.16329000 | #O |
| 1.48850000 | 1.98350000  | 15.16327000 | #O |
| 0.00010000 | 6.51016000  | 13.88570000 | #O |
| 0.00003000 | 3.25505000  | 13.18501000 | #O |
| 1.48830000 | 1.27528000  | 11.90725000 | #O |
| 1.48825000 | 5.23486000  | 11.90720000 | #O |
| 5.95309900 | 3.25511000  | 10.62987000 | #O |
| 0.00002000 | 0.00006000  | 9.93115000  | #O |
| 1.48841000 | 4.52691000  | 8.65098000  | #O |
| 1.48816000 | 1.98319000  | 8.65095000  | #O |
| 0.00008000 | 13.02034200 | 7.38649000  | #O |
| 0.00011000 | 3.25510000  | 6.65714000  | #O |
| 1.48825000 | 1.29279000  | 5.40047000  | #O |
| 1.48829000 | 5.21739000  | 5.40050000  | #O |
| 0.00007000 | 3.25516000  | 4.05392000  | #O |
| 0.00031000 | 0.00016000  | 3.49878000  | #O |
| 1.48777000 | 4.44008000  | 2.10223000  | #O |
| 1.48888000 | 2.07024000  | 2.10232000  | #O |
| 5.95309900 | 13.02014200 | 0.95207000  | #O |
| 5.95212900 | 6.51995000  | 22.88197000 | #O |
| 1.49419000 | 10.96038000 | 21.70672000 | #O |

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|------------|-------------|-------------|----|
| 1.49785000 | 8.56708000  | 21.70441000 | #O |
| 0.00026000 | 0.00133000  | 20.31830000 | #O |
| 5.95304900 | 9.76466000  | 19.74212000 | #O |
| 1.48848000 | 7.80018000  | 18.41360000 | #O |
| 1.48845000 | 11.73111000 | 18.41373000 | #O |
| 5.95309900 | 9.76564000  | 17.15662000 | #O |
| 5.95312900 | 6.50988000  | 16.43009000 | #O |
| 1.48796000 | 11.03782000 | 15.16265000 | #O |
| 1.48878000 | 8.49339000  | 15.16250000 | #O |
| 0.00003000 | 0.00000000  | 13.88588000 | #O |
| 5.95309900 | 9.76526000  | 13.18656000 | #O |
| 1.48826000 | 7.78519000  | 11.90708000 | #O |
| 1.48829000 | 11.74555000 | 11.90710000 | #O |
| 0.00002000 | 9.76555000  | 10.63075000 | #O |
| 0.00002000 | 6.51028000  | 9.93106000  | #O |
| 1.48839000 | 11.03765000 | 8.65035000  | #O |
| 1.48808000 | 8.49311000  | 8.65037000  | #O |
| 5.95305900 | 6.51039000  | 7.38649000  | #O |
| 0.00000000 | 9.76546000  | 6.65463000  | #O |
| 1.48837000 | 7.80291000  | 5.40039000  | #O |
| 1.48820000 | 11.72774000 | 5.40037000  | #O |
| 5.95311900 | 9.76529000  | 4.05682000  | #O |
| 5.95310900 | 6.50997000  | 3.49838000  | #O |
| 1.48769000 | 10.94947000 | 2.10207000  | #O |
| 1.48888000 | 8.58113000  | 2.10184000  | #O |
| 0.00011000 | 6.51061000  | 0.95171000  | #O |
| 2.97588000 | 0.00202000  | 22.85684000 | #O |
| 4.46552000 | 4.44312000  | 21.70927000 | #O |
| 4.46472000 | 2.06778000  | 21.70887000 | #O |
| 2.97630000 | 6.50865000  | 20.31900000 | #O |
| 2.97667000 | 3.25503000  | 19.75832000 | #O |
| 4.46495000 | 1.29296000  | 18.41389000 | #O |
| 4.46499000 | 5.21649000  | 18.41377000 | #O |
| 2.97651000 | 3.25504000  | 17.15732000 | #O |
| 2.97662000 | 0.00032000  | 16.43027000 | #O |
| 4.46481000 | 4.52610000  | 15.16330000 | #O |
| 4.46498000 | 1.98385000  | 15.16317000 | #O |
| 2.97661000 | 6.51017000  | 13.88559000 | #O |
| 2.97662000 | 3.25507000  | 13.18504000 | #O |
| 4.46486000 | 1.27525000  | 11.90722000 | #O |
| 4.46487000 | 5.23490000  | 11.90718000 | #O |
| 2.97667000 | 3.25507000  | 10.62980000 | #O |
| 2.97661000 | 0.00002000  | 9.93117000  | #O |
| 4.46502000 | 4.52681000  | 8.65100000  | #O |
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