

## Supporting Information

### Selective Noble Gas Inclusion in Pentagon-Dodecahedral X<sub>20</sub>-Cages

Christopher Weinert <sup>1</sup>, Dušan Čoćić <sup>2</sup>, Ralph Puchta <sup>1,3,4,5,\*</sup> and Rudi van Eldik <sup>3,6,\*</sup>

<sup>1</sup> Fakultät Angewandte Mathematik, Physik und Allgemeinwissenschaften, Technische Hochschule Nuremberg Georg Simon Ohm, Keßlerplatz 12, 90489 Nuremberg, Germany

<sup>2</sup> Department of Chemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, P.O. Box 60, 34000 Kragujevac, Serbia

<sup>3</sup> Inorganic Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Egerlandstr. 1, 91058 Erlangen, Germany

<sup>4</sup> Central Institute for Scientific Computing (CISC), University of Erlangen-Nuremberg, Martensstr. 5a, 91058 Erlangen, Germany

<sup>5</sup> Computer Chemistry Center, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Nögelsbachstr. 25, 91052 Erlangen, Germany

<sup>6</sup> Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

\* Correspondence: ralph.puchta@fau.de (R.P.); rudi.vaneldik@fau.de (R.v.E.)

† Dedicated to Prof. Dr. Thomas Lauterbach on the Occasion of his 60th birthday.

Table S1. Optimized ( $\omega$ B97XD/ def2-svp/svpfit) XYZ coordinates of the structures reported in the manuscript.

C<sub>20</sub>H<sub>20</sub>

C -1.252105 -0.406833 1.723374  
C 1.252105 1.723374 0.406833  
C 1.252105 -1.723374 -0.406833  
C 1.252105 -0.406833 1.723374  
C 0.000000 -2.130208 0.406833  
C -0.773843 1.065104 1.723374  
C 2.025948 0.658270 -0.406833  
C 0.000000 2.130208 -0.406833  
C 0.773843 -1.065104 -1.723374  
C -2.025948 -0.658270 0.406833  
C 1.252105 0.406833 -1.723374  
C -1.252105 -1.723374 -0.406833  
C -1.252105 1.723374 0.406833  
C -1.252105 0.406833 -1.723374  
C -0.773843 -1.065104 -1.723374  
C -2.025948 0.658270 -0.406833  
C -0.000000 1.316541 -1.723374  
C 2.025948 -0.658270 0.406833  
C -0.000000 -1.316541 1.723374  
C 0.773843 1.065104 1.723374  
H 0.000000 3.209823 -0.613022  
H 1.166036 -1.604911 -2.596801  
H -3.052723 -0.991890 0.613022  
H 1.886687 0.613022 -2.596801  
H -1.886687 -2.596801 -0.613022  
H -1.886687 2.596801 0.613022  
H -1.886687 0.613022 -2.596801

H -1.166036 -1.604911 -2.596801  
 H -3.052723 0.991890 -0.613022  
 H -0.000000 1.983780 -2.596801  
 H 3.052723 0.991890 -0.613022  
 H 0.000000 -3.209823 0.613022  
 H -1.166036 1.604911 2.596801  
 H -1.886687 -0.613022 2.596801  
 H 1.886687 2.596801 0.613022  
 H 1.886687 -2.596801 -0.613022  
 H 1.886687 -0.613022 2.596801  
 H -0.000000 -1.983780 2.596801  
 H 1.166036 1.604911 2.596801  
 H 3.052723 -0.991890 0.613022

C<sub>20</sub>H<sub>20</sub> ⊂ He

He 0.000000 0.000000 0.000000  
 C -1.258861 -0.409029 1.732673  
 C 1.258861 1.732673 0.409029  
 C 1.258861 -1.732673 -0.409029  
 C 1.258861 -0.409029 1.732673  
 C -0.000000 -2.141701 0.409029  
 C -0.778019 1.070851 1.732673  
 C 2.036879 0.661822 -0.409029  
 C -0.000000 2.141701 -0.409029  
 C 0.778019 -1.070851 -1.732673  
 C -2.036879 -0.661822 0.409029  
 C 1.258861 0.409029 -1.732673  
 C -1.258861 -1.732673 -0.409029  
 C -1.258861 1.732673 0.409029  
 C -1.258861 0.409029 -1.732673

C -0.778019 -1.070851 -1.732673  
 C -2.036879 0.661822 -0.409029  
 C -0.000000 1.323644 -1.732673  
 C 2.036879 -0.661822 0.409029  
 C -0.000000 -1.323644 1.732673  
 C 0.778019 1.070851 1.732673  
 H -0.000000 3.220980 -0.615152  
 H 1.170089 -1.610490 -2.605827  
 H -3.063334 -0.995338 0.615152  
 H 1.893244 0.615152 -2.605827  
 H -1.893244 -2.605827 -0.615152  
 H -1.893244 2.605827 0.615152  
 H -1.893244 0.615152 -2.605827  
 H -1.170089 -1.610490 -2.605827  
 H -3.063334 0.995338 -0.615152  
 H -0.000000 1.990675 -2.605827  
 H 3.063334 0.995338 -0.615152  
 H -0.000000 -3.220980 0.615152  
 H -1.170089 1.610490 2.605827  
 H -1.893244 -0.615152 2.605827  
 H 1.893244 2.605827 0.615152  
 H 1.893244 -2.605827 -0.615152  
 H 1.893244 -0.615152 2.605827  
 H -0.000000 -1.990675 2.605827  
 H 1.170089 1.610490 2.605827  
 H 3.063334 -0.995338 0.615152

$C_{20}H_{20} \subset Ne$

Ne 0.000000 0.000000 0.000000  
 C -1.271734 -0.413211 1.750392

C 1.271734 1.750392 0.413211  
C 1.271734 -1.750392 -0.413211  
C 1.271734 -0.413211 1.750392  
C 0.000000 -2.163603 0.413211  
C -0.785975 1.081801 1.750392  
C 2.057709 0.668590 -0.413211  
C 0.000000 2.163603 -0.413211  
C 0.785975 -1.081801 -1.750392  
C -2.057709 -0.668590 0.413211  
C 1.271734 0.413211 -1.750392  
C -1.271734 -1.750392 -0.413211  
C -1.271734 1.750392 0.413211  
C -1.271734 0.413211 -1.750392  
C -0.785975 -1.081801 -1.750392  
C -2.057709 0.668590 -0.413211  
C 0.000000 1.337180 -1.750392  
C 2.057709 -0.668590 0.413211  
C -0.000000 -1.337180 1.750392  
C 0.785975 1.081801 1.750392  
H 0.000000 3.242417 -0.619246  
H 1.177877 -1.621208 -2.623170  
H -3.083721 -1.001962 0.619246  
H 1.905845 0.619246 -2.623170  
H -1.905845 -2.623170 -0.619246  
H -1.905845 2.623170 0.619246  
H -1.905845 0.619246 -2.623170  
H -1.177877 -1.621208 -2.623170  
H -3.083721 1.001962 -0.619246  
H 0.000000 2.003924 -2.623170  
H 3.083721 1.001962 -0.619246  
H 0.000000 -3.242417 0.619246

H -1.177877 1.621208 2.623170  
H -1.905845 -0.619246 2.623170  
H 1.905845 2.623170 0.619246  
H 1.905845 -2.623170 -0.619246  
H 1.905845 -0.619246 2.623170  
H -0.000000 -2.003924 2.623170  
H 1.177877 1.621208 2.623170  
H 3.083721 -1.001962 0.619246

$\text{C}_{20}\text{H}_{20} \subset \text{Ar}$

Ar 0.000000 0.000000 0.000000  
C -1.304012 -0.423699 1.794819  
C 1.304012 1.794819 0.423699  
C 1.304012 -1.794819 -0.423699  
C 1.304012 -0.423699 1.794819  
C -0.000000 -2.218518 0.423699  
C -0.805924 1.109259 1.794819  
C 2.109936 0.685560 -0.423699  
C 0.000000 2.218518 -0.423699  
C 0.805924 -1.109259 -1.794819  
C -2.109936 -0.685560 0.423699  
C 1.304012 0.423699 -1.794819  
C -1.304012 -1.794819 -0.423699  
C -1.304012 1.794819 0.423699  
C -1.304012 0.423699 -1.794819  
C -0.805924 -1.109259 -1.794819  
C -2.109936 0.685560 -0.423699  
C 0.000000 1.371119 -1.794819  
C 2.109936 -0.685560 0.423699  
C -0.000000 -1.371119 1.794819

C 0.805924 1.109259 1.794819  
 H 0.000000 3.299477 -0.630144  
 H 1.198605 -1.649738 -2.669333  
 H -3.137989 -1.019594 0.630144  
 H 1.939384 0.630144 -2.669333  
 H -1.939384 -2.669333 -0.630144  
 H -1.939384 2.669333 0.630144  
 H -1.939384 0.630144 -2.669333  
 H -1.198605 -1.649738 -2.669333  
 H -3.137989 1.019594 -0.630144  
 H 0.000000 2.039189 -2.669333  
 H 3.137989 1.019594 -0.630144  
 H -0.000000 -3.299477 0.630144  
 H -1.198605 1.649738 2.669333  
 H -1.939384 -0.630144 2.669333  
 H 1.939384 2.669333 0.630144  
 H 1.939384 -2.669333 -0.630144  
 H 1.939384 -0.630144 2.669333  
 H -0.000000 -2.039189 2.669333  
 H 1.198605 1.649738 2.669333  
 H 3.137989 -1.019594 0.630144

$C_{20}H_{20} \subset Kr$

Kr 0.000000 0.000000 0.000000  
 C -1.32186 -0.429498 1.819384  
 C 1.32186 1.819384 0.429498  
 C 1.32186 -1.819384 -0.429498  
 C 1.32186 -0.429498 1.819384  
 C 0 -2.248882 0.429498  
 C -0.816954 1.124441 1.819384

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.138814  | 0.694943  | -0.429498 |
| C | 0         | 2.248882  | -0.429498 |
| C | 0.816954  | -1.124441 | -1.819384 |
| C | -2.138814 | -0.694943 | 0.429498  |
| C | 1.32186   | 0.429498  | -1.819384 |
| C | -1.32186  | -1.819384 | -0.429498 |
| C | -1.32186  | 1.819384  | 0.429498  |
| C | -1.32186  | 0.429498  | -1.819384 |
| C | -0.816954 | -1.124441 | -1.819384 |
| C | -2.138814 | 0.694943  | -0.429498 |
| C | 0         | 1.389886  | -1.819384 |
| C | 2.138814  | -0.694943 | 0.429498  |
| C | 0         | -1.389886 | 1.819384  |
| C | 0.816954  | 1.124441  | 1.819384  |
| H | 0         | 3.332732  | -0.636495 |
| H | 1.210686  | -1.666366 | -2.696237 |
| H | -3.169616 | -1.029871 | 0.636495  |
| H | 1.958931  | 0.636495  | -2.696237 |
| H | -1.958931 | -2.696237 | -0.636495 |
| H | -1.958931 | 2.696237  | 0.636495  |
| H | -1.958931 | 0.636495  | -2.696237 |
| H | -1.210686 | -1.666366 | -2.696237 |
| H | -3.169616 | 1.029871  | -0.636495 |
| H | 0         | 2.059742  | -2.696237 |
| H | 3.169616  | 1.029871  | -0.636495 |
| H | 0         | -3.332732 | 0.636495  |
| H | -1.210686 | 1.666366  | 2.696237  |
| H | -1.958931 | -0.636495 | 2.696237  |
| H | 1.958931  | 2.696237  | 0.636495  |
| H | 1.958931  | -2.696237 | -0.636495 |
| H | 1.958931  | -0.636495 | 2.696237  |

|            |           |          |  |
|------------|-----------|----------|--|
| H 0        | -2.059742 | 2.696237 |  |
| H 1.210686 | 1.666366  | 2.696237 |  |
| H 3.169616 | -1.029871 | 0.636495 |  |

C<sub>20</sub>H<sub>20</sub> ⊂ Xe

|    |           |           |           |
|----|-----------|-----------|-----------|
| Xe | 0         | 0         | 0         |
| C  | -1.342418 | -0.436178 | 1.847679  |
| C  | 1.342418  | 1.847679  | 0.436178  |
| C  | 1.342418  | -1.847679 | -0.436178 |
| C  | 1.342418  | -0.436178 | 1.847679  |
| C  | 0         | -2.283857 | 0.436178  |
| C  | -0.82966  | 1.141929  | 1.847679  |
| C  | 2.172077  | 0.705751  | -0.436178 |
| C  | 0         | 2.283857  | -0.436178 |
| C  | 0.82966   | -1.141929 | -1.847679 |
| C  | -2.172077 | -0.705751 | 0.436178  |
| C  | 1.342418  | 0.436178  | -1.847679 |
| C  | -1.342418 | -1.847679 | -0.436178 |
| C  | -1.342418 | 1.847679  | 0.436178  |
| C  | -1.342418 | 0.436178  | -1.847679 |
| C  | -0.82966  | -1.141929 | -1.847679 |
| C  | -2.172077 | 0.705751  | -0.436178 |
| C  | 0         | 1.411501  | -1.847679 |
| C  | 2.172077  | -0.705751 | 0.436178  |
| C  | 0         | -1.411501 | 1.847679  |
| C  | 0.82966   | 1.141929  | 1.847679  |
| H  | 0         | 3.372623  | -0.644114 |
| H  | 1.225177  | -1.686312 | -2.728509 |
| H  | -3.207555 | -1.042198 | 0.644114  |
| H  | 1.982378  | 0.644114  | -2.728509 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.982378 | -2.728509 | -0.644114 |
| H | -1.982378 | 2.728509  | 0.644114  |
| H | -1.982378 | 0.644114  | -2.728509 |
| H | -1.225177 | -1.686312 | -2.728509 |
| H | -3.207555 | 1.042198  | -0.644114 |
| H | 0         | 2.084396  | -2.728509 |
| H | 3.207555  | 1.042198  | -0.644114 |
| H | 0         | -3.372623 | 0.644114  |
| H | -1.225177 | 1.686312  | 2.728509  |
| H | -1.982378 | -0.644114 | 2.728509  |
| H | 1.982378  | 2.728509  | 0.644114  |
| H | 1.982378  | -2.728509 | -0.644114 |
| H | 1.982378  | -0.644114 | 2.728509  |
| H | 0         | -2.084396 | 2.728509  |
| H | 1.225177  | 1.686312  | 2.728509  |
| H | 3.207555  | -1.042198 | 0.644114  |

$C_{20}H_{20} \subset R_n$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| C  | -1.355594 | -0.440459 | 1.865815  |
| C  | 1.355594  | 1.865815  | 0.440459  |
| C  | 1.355594  | -1.865815 | -0.440459 |
| C  | 1.355594  | -0.440459 | 1.865815  |
| C  | 0         | -2.306274 | 0.440459  |
| C  | -0.837803 | 1.153137  | 1.865815  |
| C  | 2.193397  | 0.712678  | -0.440459 |
| C  | 0         | 2.306274  | -0.440459 |
| C  | 0.837803  | -1.153137 | -1.865815 |
| C  | -2.193397 | -0.712678 | 0.440459  |
| C  | 1.355594  | 0.440459  | -1.865815 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.355594 | -1.865815 | -0.440459 |
| C | -1.355594 | 1.865815  | 0.440459  |
| C | -1.355594 | 0.440459  | -1.865815 |
| C | -0.837803 | -1.153137 | -1.865815 |
| C | -2.193397 | 0.712678  | -0.440459 |
| C | 0         | 1.425356  | -1.865815 |
| C | 2.193397  | -0.712678 | 0.440459  |
| C | 0         | -1.425356 | 1.865815  |
| C | 0.837803  | 1.153137  | 1.865815  |
| H | 0         | 3.397076  | -0.648784 |
| H | 1.23406   | -1.698538 | -2.748292 |
| H | -3.230811 | -1.049754 | 0.648784  |
| H | 1.996751  | 0.648784  | -2.748292 |
| H | -1.996751 | -2.748292 | -0.648784 |
| H | -1.996751 | 2.748292  | 0.648784  |
| H | -1.996751 | 0.648784  | -2.748292 |
| H | -1.23406  | -1.698538 | -2.748292 |
| H | -3.230811 | 1.049754  | -0.648784 |
| H | 0         | 2.099508  | -2.748292 |
| H | 3.230811  | 1.049754  | -0.648784 |
| H | 0         | -3.397076 | 0.648784  |
| H | -1.23406  | 1.698538  | 2.748292  |
| H | -1.996751 | -0.648784 | 2.748292  |
| H | 1.996751  | 2.748292  | 0.648784  |
| H | 1.996751  | -2.748292 | -0.648784 |
| H | 1.996751  | -0.648784 | 2.748292  |
| H | 0         | -2.099508 | 2.748292  |
| H | 1.23406   | 1.698538  | 2.748292  |
| H | 3.230811  | -1.049754 | 0.648784  |

Si<sub>20</sub>H<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | -1.914952 | -0.622206 | 2.635706  |
| Si | 1.914952  | 2.635706  | 0.622206  |
| Si | 1.914952  | -2.635706 | -0.622206 |
| Si | 1.914952  | -0.622206 | 2.635706  |
| Si | 0         | -3.257912 | 0.622206  |
| Si | -1.183506 | 1.628956  | 2.635706  |
| Si | 3.098458  | 1.00675   | -0.622206 |
| Si | 0         | 3.257912  | -0.622206 |
| Si | 1.183506  | -1.628956 | -2.635706 |
| Si | -3.098458 | -1.00675  | 0.622206  |
| Si | 1.914952  | 0.622206  | -2.635706 |
| Si | -1.914952 | -2.635706 | -0.622206 |
| Si | -1.914952 | 2.635706  | 0.622206  |
| Si | -1.914952 | 0.622206  | -2.635706 |
| Si | -1.183506 | -1.628956 | -2.635706 |
| Si | -3.098458 | 1.00675   | -0.622206 |
| Si | 0         | 2.0135    | -2.635706 |
| Si | 3.098458  | -1.00675  | 0.622206  |
| Si | 0         | -2.0135   | 2.635706  |
| Si | 1.183506  | 1.628956  | 2.635706  |
| H  | 0         | 4.726497  | -0.902681 |
| H  | 1.717     | -2.363248 | -3.823816 |
| H  | -4.495165 | -1.460568 | 0.902681  |
| H  | 2.778165  | 0.902681  | -3.823816 |
| H  | -2.778165 | -3.823816 | -0.902681 |
| H  | -2.778165 | 3.823816  | 0.902681  |
| H  | -2.778165 | 0.902681  | -3.823816 |
| H  | -1.717    | -2.363248 | -3.823816 |
| H  | -4.495165 | 1.460568  | -0.902681 |
| H  | 0         | 2.921136  | -3.823816 |
| H  | 4.495165  | 1.460568  | -0.902681 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0         | -4.726497 | 0.902681  |
| H | -1.717    | 2.363248  | 3.823816  |
| H | -2.778165 | -0.902681 | 3.823816  |
| H | 2.778165  | 3.823816  | 0.902681  |
| H | 2.778165  | -3.823816 | -0.902681 |
| H | 2.778165  | -0.902681 | 3.823816  |
| H | 0         | -2.921136 | 3.823816  |
| H | 1.717     | 2.363248  | 3.823816  |
| H | 4.495165  | -1.460568 | 0.902681  |

Si<sub>20</sub>H<sub>20</sub> ⊂ He

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Si | -1.915933 | -0.622525 | 2.637056  |
| Si | 1.915933  | 2.637056  | 0.622525  |
| Si | 1.915933  | -2.637056 | -0.622525 |
| Si | 1.915933  | -0.622525 | 2.637056  |
| Si | 0         | -3.259581 | 0.622525  |
| Si | -1.184112 | 1.62979   | 2.637056  |
| Si | 3.100045  | 1.007266  | -0.622525 |
| Si | 0         | 3.259581  | -0.622525 |
| Si | 1.184112  | -1.62979  | -2.637056 |
| Si | -3.100045 | -1.007266 | 0.622525  |
| Si | 1.915933  | 0.622525  | -2.637056 |
| Si | -1.915933 | -2.637056 | -0.622525 |
| Si | -1.915933 | 2.637056  | 0.622525  |
| Si | -1.915933 | 0.622525  | -2.637056 |
| Si | -1.184112 | -1.62979  | -2.637056 |
| Si | -3.100045 | 1.007266  | -0.622525 |
| Si | 0         | 2.014532  | -2.637056 |
| Si | 3.100045  | -1.007266 | 0.622525  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | 0         | -2.014532 | 2.637056  |
| Si | 1.184112  | 1.62979   | 2.637056  |
| H  | 0         | 4.727809  | -0.902931 |
| H  | 1.717477  | -2.363905 | -3.824878 |
| H  | -4.496414 | -1.460973 | 0.902931  |
| H  | 2.778936  | 0.902931  | -3.824878 |
| H  | -2.778936 | -3.824878 | -0.902931 |
| H  | -2.778936 | 3.824878  | 0.902931  |
| H  | -2.778936 | 0.902931  | -3.824878 |
| H  | -1.717477 | -2.363905 | -3.824878 |
| H  | -4.496414 | 1.460973  | -0.902931 |
| H  | 0         | 2.921947  | -3.824878 |
| H  | 4.496414  | 1.460973  | -0.902931 |
| H  | 0         | -4.727809 | 0.902931  |
| H  | -1.717477 | 2.363905  | 3.824878  |
| H  | -2.778936 | -0.902931 | 3.824878  |
| H  | 2.778936  | 3.824878  | 0.902931  |
| H  | 2.778936  | -3.824878 | -0.902931 |
| H  | 2.778936  | -0.902931 | 3.824878  |
| H  | 0         | -2.921947 | 3.824878  |
| H  | 1.717477  | 2.363905  | 3.824878  |
| H  | 4.496414  | -1.460973 | 0.902931  |

Si<sub>20</sub>H<sub>20</sub> ⊂ Ne

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ne | 0         | 0         | 0         |
| Si | -1.917032 | -0.622881 | 2.638568  |
| Si | 1.917032  | 2.638568  | 0.622881  |
| Si | 1.917032  | -2.638568 | -0.622881 |
| Si | 1.917032  | -0.622881 | 2.638568  |
| Si | 0         | -3.261449 | 0.622881  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | -1.184791 | 1.630725  | 2.638568  |
| Si | 3.101823  | 1.007843  | -0.622881 |
| Si | 0         | 3.261449  | -0.622881 |
| Si | 1.184791  | -1.630725 | -2.638568 |
| Si | -3.101823 | -1.007843 | 0.622881  |
| Si | 1.917032  | 0.622881  | -2.638568 |
| Si | -1.917032 | -2.638568 | -0.622881 |
| Si | -1.917032 | 2.638568  | 0.622881  |
| Si | -1.917032 | 0.622881  | -2.638568 |
| Si | -1.184791 | -1.630725 | -2.638568 |
| Si | -3.101823 | 1.007843  | -0.622881 |
| Si | 0         | 2.015687  | -2.638568 |
| Si | 3.101823  | -1.007843 | 0.622881  |
| Si | 0         | -2.015687 | 2.638568  |
| Si | 1.184791  | 1.630725  | 2.638568  |
| H  | 0         | 4.729535  | -0.903261 |
| H  | 1.718104  | -2.364768 | -3.826275 |
| H  | -4.498056 | -1.461507 | 0.903261  |
| H  | 2.779951  | 0.903261  | -3.826275 |
| H  | -2.779951 | -3.826275 | -0.903261 |
| H  | -2.779951 | 3.826275  | 0.903261  |
| H  | -2.779951 | 0.903261  | -3.826275 |
| H  | -1.718104 | -2.364768 | -3.826275 |
| H  | -4.498056 | 1.461507  | -0.903261 |
| H  | 0         | 2.923014  | -3.826275 |
| H  | 4.498056  | 1.461507  | -0.903261 |
| H  | 0         | -4.729535 | 0.903261  |
| H  | -1.718104 | 2.364768  | 3.826275  |
| H  | -2.779951 | -0.903261 | 3.826275  |
| H  | 2.779951  | 3.826275  | 0.903261  |
| H  | 2.779951  | -3.826275 | -0.903261 |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 2.779951 | -0.903261 | 3.826275 |
| H | 0        | -2.923014 | 3.826275 |
| H | 1.718104 | 2.364768  | 3.826275 |
| H | 4.498056 | -1.461507 | 0.903261 |

Si<sub>20</sub>H<sub>20</sub> ⊂ Ar

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ar | 0         | 0         | 0         |
| Si | -1.923931 | -0.625123 | 2.648064  |
| Si | 1.923931  | 2.648064  | 0.625123  |
| Si | 1.923931  | -2.648064 | -0.625123 |
| Si | 1.923931  | -0.625123 | 2.648064  |
| Si | 0         | -3.273187 | 0.625123  |
| Si | -1.189055 | 1.636593  | 2.648064  |
| Si | 3.112986  | 1.01147   | -0.625123 |
| Si | 0         | 3.273187  | -0.625123 |
| Si | 1.189055  | -1.636593 | -2.648064 |
| Si | -3.112986 | -1.01147  | 0.625123  |
| Si | 1.923931  | 0.625123  | -2.648064 |
| Si | -1.923931 | -2.648064 | -0.625123 |
| Si | -1.923931 | 2.648064  | 0.625123  |
| Si | -1.923931 | 0.625123  | -2.648064 |
| Si | -1.189055 | -1.636593 | -2.648064 |
| Si | -3.112986 | 1.01147   | -0.625123 |
| Si | 0         | 2.022941  | -2.648064 |
| Si | 3.112986  | -1.01147  | 0.625123  |
| Si | 0         | -2.022941 | 2.648064  |
| Si | 1.189055  | 1.636593  | 2.648064  |
| H  | 0         | 4.740989  | -0.905448 |
| H  | 1.722265  | -2.370495 | -3.835541 |
| H  | -4.508949 | -1.465046 | 0.905448  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.786683  | 0.905448  | -3.835541 |
| H | -2.786683 | -3.835541 | -0.905448 |
| H | -2.786683 | 3.835541  | 0.905448  |
| H | -2.786683 | 0.905448  | -3.835541 |
| H | -1.722265 | -2.370495 | -3.835541 |
| H | -4.508949 | 1.465046  | -0.905448 |
| H | 0         | 2.930092  | -3.835541 |
| H | 4.508949  | 1.465046  | -0.905448 |
| H | 0         | -4.740989 | 0.905448  |
| H | -1.722265 | 2.370495  | 3.835541  |
| H | -2.786683 | -0.905448 | 3.835541  |
| H | 2.786683  | 3.835541  | 0.905448  |
| H | 2.786683  | -3.835541 | -0.905448 |
| H | 2.786683  | -0.905448 | 3.835541  |
| H | 0         | -2.930092 | 3.835541  |
| H | 1.722265  | 2.370495  | 3.835541  |
| H | 4.508949  | -1.465046 | 0.905448  |

Si<sub>20</sub>H<sub>20</sub> ⊂ Kr

|    |           |           |           |
|----|-----------|-----------|-----------|
| Kr | 0         | 0         | 0         |
| Si | -1.931114 | -0.627457 | 2.657951  |
| Si | 1.931114  | 2.657951  | 0.627457  |
| Si | 1.931114  | -2.657951 | -0.627457 |
| Si | 1.931114  | -0.627457 | 2.657951  |
| Si | 0         | -3.285408 | 0.627457  |
| Si | -1.193494 | 1.642704  | 2.657951  |
| Si | 3.124608  | 1.015247  | -0.627457 |
| Si | 0         | 3.285408  | -0.627457 |
| Si | 1.193494  | -1.642704 | -2.657951 |
| Si | -3.124608 | -1.015247 | 0.627457  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | 1.931114  | 0.627457  | -2.657951 |
| Si | -1.931114 | -2.657951 | -0.627457 |
| Si | -1.931114 | 2.657951  | 0.627457  |
| Si | -1.931114 | 0.627457  | -2.657951 |
| Si | -1.193494 | -1.642704 | -2.657951 |
| Si | -3.124608 | 1.015247  | -0.627457 |
| Si | 0         | 2.030494  | -2.657951 |
| Si | 3.124608  | -1.015247 | 0.627457  |
| Si | 0         | -2.030494 | 2.657951  |
| Si | 1.193494  | 1.642704  | 2.657951  |
| H  | 0         | 4.753216  | -0.907783 |
| H  | 1.726707  | -2.376608 | -3.845432 |
| H  | -4.520577 | -1.468824 | 0.907783  |
| H  | 2.79387   | 0.907783  | -3.845432 |
| H  | -2.79387  | -3.845432 | -0.907783 |
| H  | -2.79387  | 3.845432  | 0.907783  |
| H  | -2.79387  | 0.907783  | -3.845432 |
| H  | -1.726707 | -2.376608 | -3.845432 |
| H  | -4.520577 | 1.468824  | -0.907783 |
| H  | 0         | 2.937649  | -3.845432 |
| H  | 4.520577  | 1.468824  | -0.907783 |
| H  | 0         | -4.753216 | 0.907783  |
| H  | -1.726707 | 2.376608  | 3.845432  |
| H  | -2.79387  | -0.907783 | 3.845432  |
| H  | 2.79387   | 3.845432  | 0.907783  |
| H  | 2.79387   | -3.845432 | -0.907783 |
| H  | 2.79387   | -0.907783 | 3.845432  |
| H  | 0         | -2.937649 | 3.845432  |
| H  | 1.726707  | 2.376608  | 3.845432  |
| H  | 4.520577  | -1.468824 | 0.907783  |

Si<sub>20</sub>H<sub>20</sub> ⊂ Xe

|    |           |           |           |
|----|-----------|-----------|-----------|
| Xe | 0         | 0         | 0         |
| Si | -1.939288 | -0.630113 | 2.669201  |
| Si | 1.939288  | 2.669201  | 0.630113  |
| Si | 1.939288  | -2.669201 | -0.630113 |
| Si | 1.939288  | -0.630113 | 2.669201  |
| Si | 0         | -3.299314 | 0.630113  |
| Si | -1.198546 | 1.649657  | 2.669201  |
| Si | 3.137834  | 1.019544  | -0.630113 |
| Si | 0         | 3.299314  | -0.630113 |
| Si | 1.198546  | -1.649657 | -2.669201 |
| Si | -3.137834 | -1.019544 | 0.630113  |
| Si | 1.939288  | 0.630113  | -2.669201 |
| Si | -1.939288 | -2.669201 | -0.630113 |
| Si | -1.939288 | 2.669201  | 0.630113  |
| Si | -1.939288 | 0.630113  | -2.669201 |
| Si | -1.198546 | -1.649657 | -2.669201 |
| Si | -3.137834 | 1.019544  | -0.630113 |
| Si | 0         | 2.039088  | -2.669201 |
| Si | 3.137834  | -1.019544 | 0.630113  |
| Si | 0         | -2.039088 | 2.669201  |
| Si | 1.198546  | 1.649657  | 2.669201  |
| H  | 0         | 4.767448  | -0.910502 |
| H  | 1.731877  | -2.383724 | -3.856947 |
| H  | -4.534113 | -1.473222 | 0.910502  |
| H  | 2.802236  | 0.910502  | -3.856947 |
| H  | -2.802236 | -3.856947 | -0.910502 |
| H  | -2.802236 | 3.856947  | 0.910502  |
| H  | -2.802236 | 0.910502  | -3.856947 |
| H  | -1.731877 | -2.383724 | -3.856947 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.534113 | 1.473222  | -0.910502 |
| H | 0         | 2.946445  | -3.856947 |
| H | 4.534113  | 1.473222  | -0.910502 |
| H | 0         | -4.767448 | 0.910502  |
| H | -1.731877 | 2.383724  | 3.856947  |
| H | -2.802236 | -0.910502 | 3.856947  |
| H | 2.802236  | 3.856947  | 0.910502  |
| H | 2.802236  | -3.856947 | -0.910502 |
| H | 2.802236  | -0.910502 | 3.856947  |
| H | 0         | -2.946445 | 3.856947  |
| H | 1.731877  | 2.383724  | 3.856947  |
| H | 4.534113  | -1.473222 | 0.910502  |

Si<sub>20</sub>H<sub>20</sub>  $\subset$  Rn

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Si | -1.942698 | -0.631221 | 2.673894  |
| Si | 1.942698  | 2.673894  | 0.631221  |
| Si | 1.942698  | -2.673894 | -0.631221 |
| Si | 1.942698  | -0.631221 | 2.673894  |
| Si | 0         | -3.305115 | 0.631221  |
| Si | -1.200653 | 1.652558  | 2.673894  |
| Si | 3.143351  | 1.021337  | -0.631221 |
| Si | 0         | 3.305115  | -0.631221 |
| Si | 1.200653  | -1.652558 | -2.673894 |
| Si | -3.143351 | -1.021337 | 0.631221  |
| Si | 1.942698  | 0.631221  | -2.673894 |
| Si | -1.942698 | -2.673894 | -0.631221 |
| Si | -1.942698 | 2.673894  | 0.631221  |
| Si | -1.942698 | 0.631221  | -2.673894 |
| Si | -1.200653 | -1.652558 | -2.673894 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | -3.143351 | 1.021337  | -0.631221 |
| Si | 0         | 2.042673  | -2.673894 |
| Si | 3.143351  | -1.021337 | 0.631221  |
| Si | 0         | -2.042673 | 2.673894  |
| Si | 1.200653  | 1.652558  | 2.673894  |
| H  | 0         | 4.773569  | -0.911671 |
| H  | 1.7341    | -2.386784 | -3.861898 |
| H  | -4.539934 | -1.475114 | 0.911671  |
| H  | 2.805833  | 0.911671  | -3.861898 |
| H  | -2.805833 | -3.861898 | -0.911671 |
| H  | -2.805833 | 3.861898  | 0.911671  |
| H  | -2.805833 | 0.911671  | -3.861898 |
| H  | -1.7341   | -2.386784 | -3.861898 |
| H  | -4.539934 | 1.475114  | -0.911671 |
| H  | 0         | 2.950228  | -3.861898 |
| H  | 4.539934  | 1.475114  | -0.911671 |
| H  | 0         | -4.773569 | 0.911671  |
| H  | -1.7341   | 2.386784  | 3.861898  |
| H  | -2.805833 | -0.911671 | 3.861898  |
| H  | 2.805833  | 3.861898  | 0.911671  |
| H  | 2.805833  | -3.861898 | -0.911671 |
| H  | 2.805833  | -0.911671 | 3.861898  |
| H  | 0         | -2.950228 | 3.861898  |
| H  | 1.7341    | 2.386784  | 3.861898  |
| H  | 4.539934  | -1.475114 | 0.911671  |

# Ge<sub>20</sub>H<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | -1.982484 | -0.644148 | 2.728655  |
| Ge | 1.982484  | 2.728655  | 0.644148  |
| Ge | 1.982484  | -2.728655 | -0.644148 |
| Ge | 1.982484  | -0.644148 | 2.728655  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | 0         | -3.372803 | 0.644148  |
| Ge | -1.225242 | 1.686401  | 2.728655  |
| Ge | 3.207726  | 1.042253  | -0.644148 |
| Ge | 0         | 3.372803  | -0.644148 |
| Ge | 1.225242  | -1.686401 | -2.728655 |
| Ge | -3.207726 | -1.042253 | 0.644148  |
| Ge | 1.982484  | 0.644148  | -2.728655 |
| Ge | -1.982484 | -2.728655 | -0.644148 |
| Ge | -1.982484 | 2.728655  | 0.644148  |
| Ge | -1.982484 | 0.644148  | -2.728655 |
| Ge | -1.225242 | -1.686401 | -2.728655 |
| Ge | -3.207726 | 1.042253  | -0.644148 |
| Ge | 0         | 2.084507  | -2.728655 |
| Ge | 3.207726  | -1.042253 | 0.644148  |
| Ge | 0         | -2.084507 | 2.728655  |
| Ge | 1.225242  | 1.686401  | 2.728655  |
| H  | 0         | 4.887037  | -0.933341 |
| H  | 1.77532   | -2.443518 | -3.953696 |
| H  | -4.647848 | -1.510177 | 0.933341  |
| H  | 2.872528  | 0.933341  | -3.953696 |
| H  | -2.872528 | -3.953696 | -0.933341 |
| H  | -2.872528 | 3.953696  | 0.933341  |
| H  | -2.872528 | 0.933341  | -3.953696 |
| H  | -1.77532  | -2.443518 | -3.953696 |
| H  | -4.647848 | 1.510177  | -0.933341 |
| H  | 0         | 3.020355  | -3.953696 |
| H  | 4.647848  | 1.510177  | -0.933341 |
| H  | 0         | -4.887037 | 0.933341  |
| H  | -1.77532  | 2.443518  | 3.953696  |
| H  | -2.872528 | -0.933341 | 3.953696  |
| H  | 2.872528  | 3.953696  | 0.933341  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 2.872528 | -3.953696 | -0.933341 |
| H | 2.872528 | -0.933341 | 3.953696  |
| H | 0        | -3.020355 | 3.953696  |
| H | 1.77532  | 2.443518  | 3.953696  |
| H | 4.647848 | -1.510177 | 0.933341  |

Ge<sub>20</sub>H<sub>20</sub> ⊂ He

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Ge | -1.983604 | -0.644512 | 2.730197  |
| Ge | 1.983604  | 2.730197  | 0.644512  |
| Ge | 1.983604  | -2.730197 | -0.644512 |
| Ge | 1.983604  | -0.644512 | 2.730197  |
| Ge | 0         | -3.374709 | 0.644512  |
| Ge | -1.225935 | 1.687355  | 2.730197  |
| Ge | 3.209539  | 1.042843  | -0.644512 |
| Ge | 0         | 3.374709  | -0.644512 |
| Ge | 1.225935  | -1.687355 | -2.730197 |
| Ge | -3.209539 | -1.042843 | 0.644512  |
| Ge | 1.983604  | 0.644512  | -2.730197 |
| Ge | -1.983604 | -2.730197 | -0.644512 |
| Ge | -1.983604 | 2.730197  | 0.644512  |
| Ge | -1.983604 | 0.644512  | -2.730197 |
| Ge | -1.225935 | -1.687355 | -2.730197 |
| Ge | -3.209539 | 1.042843  | -0.644512 |
| Ge | 0         | 2.085685  | -2.730197 |
| Ge | 3.209539  | -1.042843 | 0.644512  |
| Ge | 0         | -2.085685 | 2.730197  |
| Ge | 1.225935  | 1.687355  | 2.730197  |
| H  | 0         | 4.888794  | -0.933677 |
| H  | 1.775958  | -2.444397 | -3.955118 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.64952  | -1.51072  | 0.933677  |
| H | 2.873561  | 0.933677  | -3.955118 |
| H | -2.873561 | -3.955118 | -0.933677 |
| H | -2.873561 | 3.955118  | 0.933677  |
| H | -2.873561 | 0.933677  | -3.955118 |
| H | -1.775958 | -2.444397 | -3.955118 |
| H | -4.64952  | 1.51072   | -0.933677 |
| H | 0         | 3.021441  | -3.955118 |
| H | 4.64952   | 1.51072   | -0.933677 |
| H | 0         | -4.888794 | 0.933677  |
| H | -1.775958 | 2.444397  | 3.955118  |
| H | -2.873561 | -0.933677 | 3.955118  |
| H | 2.873561  | 3.955118  | 0.933677  |
| H | 2.873561  | -3.955118 | -0.933677 |
| H | 2.873561  | -0.933677 | 3.955118  |
| H | 0         | -3.021441 | 3.955118  |
| H | 1.775958  | 2.444397  | 3.955118  |
| H | 4.64952   | -1.51072  | 0.933677  |

Ge<sub>20</sub>H<sub>20</sub> ⊂ Ne

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ne | 0         | 0         | 0         |
| Ge | -1.984042 | -0.644654 | 2.7308    |
| Ge | 1.984042  | 2.7308    | 0.644654  |
| Ge | 1.984042  | -2.7308   | -0.644654 |
| Ge | 1.984042  | -0.644654 | 2.7308    |
| Ge | 0         | -3.375454 | 0.644654  |
| Ge | -1.226206 | 1.687727  | 2.7308    |
| Ge | 3.210248  | 1.043073  | -0.644654 |
| Ge | 0         | 3.375454  | -0.644654 |
| Ge | 1.226206  | -1.687727 | -2.7308   |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | -3.210248 | -1.043073 | 0.644654  |
| Ge | 1.984042  | 0.644654  | -2.7308   |
| Ge | -1.984042 | -2.7308   | -0.644654 |
| Ge | -1.984042 | 2.7308    | 0.644654  |
| Ge | -1.984042 | 0.644654  | -2.7308   |
| Ge | -1.226206 | -1.687727 | -2.7308   |
| Ge | -3.210248 | 1.043073  | -0.644654 |
| Ge | 0         | 2.086145  | -2.7308   |
| Ge | 3.210248  | -1.043073 | 0.644654  |
| Ge | 0         | -2.086145 | 2.7308    |
| Ge | 1.226206  | 1.687727  | 2.7308    |
| H  | 0         | 4.889469  | -0.933805 |
| H  | 1.776203  | -2.444734 | -3.955663 |
| H  | -4.650161 | -1.510929 | 0.933805  |
| H  | 2.873957  | 0.933805  | -3.955663 |
| H  | -2.873957 | -3.955663 | -0.933805 |
| H  | -2.873957 | 3.955663  | 0.933805  |
| H  | -2.873957 | 0.933805  | -3.955663 |
| H  | -1.776203 | -2.444734 | -3.955663 |
| H  | -4.650161 | 1.510929  | -0.933805 |
| H  | 0         | 3.021858  | -3.955663 |
| H  | 4.650161  | 1.510929  | -0.933805 |
| H  | 0         | -4.889469 | 0.933805  |
| H  | -1.776203 | 2.444734  | 3.955663  |
| H  | -2.873957 | -0.933805 | 3.955663  |
| H  | 2.873957  | 3.955663  | 0.933805  |
| H  | 2.873957  | -3.955663 | -0.933805 |
| H  | 2.873957  | -0.933805 | 3.955663  |
| H  | 0         | -3.021858 | 3.955663  |
| H  | 1.776203  | 2.444734  | 3.955663  |
| H  | 4.650161  | -1.510929 | 0.933805  |

Ge<sub>20</sub>H<sub>20</sub>  $\subset$  Ar

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ar | 0         | 0         | 0         |
| Ge | -1.992727 | -0.647476 | 2.742754  |
| Ge | 1.992727  | 2.742754  | 0.647476  |
| Ge | 1.992727  | -2.742754 | -0.647476 |
| Ge | 1.992727  | -0.647476 | 2.742754  |
| Ge | 0         | -3.39023  | 0.647476  |
| Ge | -1.231573 | 1.695115  | 2.742754  |
| Ge | 3.224301  | 1.047639  | -0.647476 |
| Ge | 0         | 3.39023   | -0.647476 |
| Ge | 1.231573  | -1.695115 | -2.742754 |
| Ge | -3.224301 | -1.047639 | 0.647476  |
| Ge | 1.992727  | 0.647476  | -2.742754 |
| Ge | -1.992727 | -2.742754 | -0.647476 |
| Ge | -1.992727 | 2.742754  | 0.647476  |
| Ge | -1.992727 | 0.647476  | -2.742754 |
| Ge | -1.231573 | -1.695115 | -2.742754 |
| Ge | -3.224301 | 1.047639  | -0.647476 |
| Ge | 0         | 2.095278  | -2.742754 |
| Ge | 3.224301  | -1.047639 | 0.647476  |
| Ge | 0         | -2.095278 | 2.742754  |
| Ge | 1.231573  | 1.695115  | 2.742754  |
| H  | 0         | 4.904431  | -0.936663 |
| H  | 1.781639  | -2.452215 | -3.967768 |
| H  | -4.664391 | -1.515552 | 0.936663  |
| H  | 2.882752  | 0.936663  | -3.967768 |
| H  | -2.882752 | -3.967768 | -0.936663 |
| H  | -2.882752 | 3.967768  | 0.936663  |
| H  | -2.882752 | 0.936663  | -3.967768 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.781639 | -2.452215 | -3.967768 |
| H | -4.664391 | 1.515552  | -0.936663 |
| H | 0         | 3.031105  | -3.967768 |
| H | 4.664391  | 1.515552  | -0.936663 |
| H | 0         | -4.904431 | 0.936663  |
| H | -1.781639 | 2.452215  | 3.967768  |
| H | -2.882752 | -0.936663 | 3.967768  |
| H | 2.882752  | 3.967768  | 0.936663  |
| H | 2.882752  | -3.967768 | -0.936663 |
| H | 2.882752  | -0.936663 | 3.967768  |
| H | 0         | -3.031105 | 3.967768  |
| H | 1.781639  | 2.452215  | 3.967768  |
| H | 4.664391  | -1.515552 | 0.936663  |

Ge<sub>20</sub>H<sub>20</sub> ⊂ Kr

|    |           |           |           |
|----|-----------|-----------|-----------|
| Kr | 0         | 0         | 0         |
| Ge | -1.997349 | -0.648978 | 2.749115  |
| Ge | 1.997349  | 2.749115  | 0.648978  |
| Ge | 1.997349  | -2.749115 | -0.648978 |
| Ge | 1.997349  | -0.648978 | 2.749115  |
| Ge | 0         | -3.398092 | 0.648978  |
| Ge | -1.234429 | 1.699046  | 2.749115  |
| Ge | 3.231778  | 1.050068  | -0.648978 |
| Ge | 0         | 3.398092  | -0.648978 |
| Ge | 1.234429  | -1.699046 | -2.749115 |
| Ge | -3.231778 | -1.050068 | 0.648978  |
| Ge | 1.997349  | 0.648978  | -2.749115 |
| Ge | -1.997349 | -2.749115 | -0.648978 |
| Ge | -1.997349 | 2.749115  | 0.648978  |
| Ge | -1.997349 | 0.648978  | -2.749115 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | -1.234429 | -1.699046 | -2.749115 |
| Ge | -3.231778 | 1.050068  | -0.648978 |
| Ge | 0         | 2.100137  | -2.749115 |
| Ge | 3.231778  | -1.050068 | 0.648978  |
| Ge | 0         | -2.100137 | 2.749115  |
| Ge | 1.234429  | 1.699046  | 2.749115  |
| H  | 0         | 4.912556  | -0.938215 |
| H  | 1.78459   | -2.456278 | -3.974341 |
| H  | -4.672118 | -1.518063 | 0.938215  |
| H  | 2.887528  | 0.938215  | -3.974341 |
| H  | -2.887528 | -3.974341 | -0.938215 |
| H  | -2.887528 | 3.974341  | 0.938215  |
| H  | -2.887528 | 0.938215  | -3.974341 |
| H  | -1.78459  | -2.456278 | -3.974341 |
| H  | -4.672118 | 1.518063  | -0.938215 |
| H  | 0         | 3.036127  | -3.974341 |
| H  | 4.672118  | 1.518063  | -0.938215 |
| H  | 0         | -4.912556 | 0.938215  |
| H  | -1.78459  | 2.456278  | 3.974341  |
| H  | -2.887528 | -0.938215 | 3.974341  |
| H  | 2.887528  | 3.974341  | 0.938215  |
| H  | 2.887528  | -3.974341 | -0.938215 |
| H  | 2.887528  | -0.938215 | 3.974341  |
| H  | 0         | -3.036127 | 3.974341  |
| H  | 1.78459   | 2.456278  | 3.974341  |
| H  | 4.672118  | -1.518063 | 0.938215  |

Ge<sub>20</sub>H<sub>20</sub> ⊂ Xe

|    |           |           |          |
|----|-----------|-----------|----------|
| Xe | 0         | 0         | 0        |
| Ge | -2.005428 | -0.651603 | 2.760234 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | 2.005428  | 2.760234  | 0.651603  |
| Ge | 2.005428  | -2.760234 | -0.651603 |
| Ge | 2.005428  | -0.651603 | 2.760234  |
| Ge | 0         | -3.411837 | 0.651603  |
| Ge | -1.239422 | 1.705919  | 2.760234  |
| Ge | 3.24485   | 1.054316  | -0.651603 |
| Ge | 0         | 3.411837  | -0.651603 |
| Ge | 1.239422  | -1.705919 | -2.760234 |
| Ge | -3.24485  | -1.054316 | 0.651603  |
| Ge | 2.005428  | 0.651603  | -2.760234 |
| Ge | -2.005428 | -2.760234 | -0.651603 |
| Ge | -2.005428 | 2.760234  | 0.651603  |
| Ge | -2.005428 | 0.651603  | -2.760234 |
| Ge | -1.239422 | -1.705919 | -2.760234 |
| Ge | -3.24485  | 1.054316  | -0.651603 |
| Ge | 0         | 2.108631  | -2.760234 |
| Ge | 3.24485   | -1.054316 | 0.651603  |
| Ge | 0         | -2.108631 | 2.760234  |
| Ge | 1.239422  | 1.705919  | 2.760234  |
| H  | 0         | 4.927013  | -0.940976 |
| H  | 1.789842  | -2.463507 | -3.986037 |
| H  | -4.685868 | -1.522531 | 0.940976  |
| H  | 2.896026  | 0.940976  | -3.986037 |
| H  | -2.896026 | -3.986037 | -0.940976 |
| H  | -2.896026 | 3.986037  | 0.940976  |
| H  | -2.896026 | 0.940976  | -3.986037 |
| H  | -1.789842 | -2.463507 | -3.986037 |
| H  | -4.685868 | 1.522531  | -0.940976 |
| H  | 0         | 3.045062  | -3.986037 |
| H  | 4.685868  | 1.522531  | -0.940976 |
| H  | 0         | -4.927013 | 0.940976  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.789842 | 2.463507  | 3.986037  |
| H | -2.896026 | -0.940976 | 3.986037  |
| H | 2.896026  | 3.986037  | 0.940976  |
| H | 2.896026  | -3.986037 | -0.940976 |
| H | 2.896026  | -0.940976 | 3.986037  |
| H | 0         | -3.045062 | 3.986037  |
| H | 1.789842  | 2.463507  | 3.986037  |
| H | 4.685868  | -1.522531 | 0.940976  |

$\text{Ge}_{20}\text{H}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Ge | -2.010524 | -0.653259 | 2.767248  |
| Ge | 2.010524  | 2.767248  | 0.653259  |
| Ge | 2.010524  | -2.767248 | -0.653259 |
| Ge | 2.010524  | -0.653259 | 2.767248  |
| Ge | 0         | -3.420507 | 0.653259  |
| Ge | -1.242572 | 1.710253  | 2.767248  |
| Ge | 3.253095  | 1.056995  | -0.653259 |
| Ge | 0         | 3.420507  | -0.653259 |
| Ge | 1.242572  | -1.710253 | -2.767248 |
| Ge | -3.253095 | -1.056995 | 0.653259  |
| Ge | 2.010524  | 0.653259  | -2.767248 |
| Ge | -2.010524 | -2.767248 | -0.653259 |
| Ge | -2.010524 | 2.767248  | 0.653259  |
| Ge | -2.010524 | 0.653259  | -2.767248 |
| Ge | -1.242572 | -1.710253 | -2.767248 |
| Ge | -3.253095 | 1.056995  | -0.653259 |
| Ge | 0         | 2.11399   | -2.767248 |
| Ge | 3.253095  | -1.056995 | 0.653259  |
| Ge | 0         | -2.11399  | 2.767248  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ge | 1.242572  | 1.710253  | 2.767248  |
| H  | 0         | 4.936289  | -0.942747 |
| H  | 1.793212  | -2.468145 | -3.993542 |
| H  | -4.69469  | -1.525397 | 0.942747  |
| H  | 2.901478  | 0.942747  | -3.993542 |
| H  | -2.901478 | -3.993542 | -0.942747 |
| H  | -2.901478 | 3.993542  | 0.942747  |
| H  | -2.901478 | 0.942747  | -3.993542 |
| H  | -1.793212 | -2.468145 | -3.993542 |
| H  | -4.69469  | 1.525397  | -0.942747 |
| H  | 0         | 3.050794  | -3.993542 |
| H  | 4.69469   | 1.525397  | -0.942747 |
| H  | 0         | -4.936289 | 0.942747  |
| H  | -1.793212 | 2.468145  | 3.993542  |
| H  | -2.901478 | -0.942747 | 3.993542  |
| H  | 2.901478  | 3.993542  | 0.942747  |
| H  | 2.901478  | -3.993542 | -0.942747 |
| H  | 2.901478  | -0.942747 | 3.993542  |
| H  | 0         | -3.050794 | 3.993542  |
| H  | 1.793212  | 2.468145  | 3.993542  |
| H  | 4.69469   | -1.525397 | 0.942747  |

Sn<sub>20</sub>H<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | -2.269448 | -0.737388 | 3.123627  |
| Sn | 2.269448  | 3.123627  | 0.737388  |
| Sn | 2.269448  | -3.123627 | -0.737388 |
| Sn | 2.269448  | -0.737388 | 3.123627  |
| Sn | 0         | -3.861016 | 0.737388  |
| Sn | -1.402596 | 1.930508  | 3.123627  |
| Sn | 3.672044  | 1.193119  | -0.737388 |
| Sn | 0         | 3.861016  | -0.737388 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | 1.402596  | -1.930508 | -3.123627 |
| Sn | -3.672044 | -1.193119 | 0.737388  |
| Sn | 2.269448  | 0.737388  | -3.123627 |
| Sn | -2.269448 | -3.123627 | -0.737388 |
| Sn | -2.269448 | 3.123627  | 0.737388  |
| Sn | -2.269448 | 0.737388  | -3.123627 |
| Sn | -1.402596 | -1.930508 | -3.123627 |
| Sn | -3.672044 | 1.193119  | -0.737388 |
| Sn | 0         | 2.386239  | -3.123627 |
| Sn | 3.672044  | -1.193119 | 0.737388  |
| Sn | 0         | -2.386239 | 3.123627  |
| Sn | 1.402596  | 1.930508  | 3.123627  |
| H  | 0         | 5.549564  | -1.059872 |
| H  | 2.015997  | -2.774782 | -4.489691 |
| H  | -5.277949 | -1.714909 | 1.059872  |
| H  | 3.261952  | 1.059872  | -4.489691 |
| H  | -3.261952 | -4.489691 | -1.059872 |
| H  | -3.261952 | 4.489691  | 1.059872  |
| H  | -3.261952 | 1.059872  | -4.489691 |
| H  | -2.015997 | -2.774782 | -4.489691 |
| H  | -5.277949 | 1.714909  | -1.059872 |
| H  | 0         | 3.429819  | -4.489691 |
| H  | 5.277949  | 1.714909  | -1.059872 |
| H  | 0         | -5.549564 | 1.059872  |
| H  | -2.015997 | 2.774782  | 4.489691  |
| H  | -3.261952 | -1.059872 | 4.489691  |
| H  | 3.261952  | 4.489691  | 1.059872  |
| H  | 3.261952  | -4.489691 | -1.059872 |
| H  | 3.261952  | -1.059872 | 4.489691  |
| H  | 0         | -3.429819 | 4.489691  |
| H  | 2.015997  | 2.774782  | 4.489691  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 5.277949 | -1.714909 | 1.059872 |
|---|----------|-----------|----------|

Sn<sub>20</sub>H<sub>20</sub> ⊂ He

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Sn | -2.269819 | -0.737509 | 3.124137  |
| Sn | 2.269819  | 3.124137  | 0.737509  |
| Sn | 2.269819  | -3.124137 | -0.737509 |
| Sn | 2.269819  | -0.737509 | 3.124137  |
| Sn | 0         | -3.861646 | 0.737509  |
| Sn | -1.402825 | 1.930823  | 3.124137  |
| Sn | 3.672643  | 1.193314  | -0.737509 |
| Sn | 0         | 3.861646  | -0.737509 |
| Sn | 1.402825  | -1.930823 | -3.124137 |
| Sn | -3.672643 | -1.193314 | 0.737509  |
| Sn | 2.269819  | 0.737509  | -3.124137 |
| Sn | -2.269819 | -3.124137 | -0.737509 |
| Sn | -2.269819 | 3.124137  | 0.737509  |
| Sn | -2.269819 | 0.737509  | -3.124137 |
| Sn | -1.402825 | -1.930823 | -3.124137 |
| Sn | -3.672643 | 1.193314  | -0.737509 |
| Sn | 0         | 2.386628  | -3.124137 |
| Sn | 3.672643  | -1.193314 | 0.737509  |
| Sn | 0         | -2.386628 | 3.124137  |
| Sn | 1.402825  | 1.930823  | 3.124137  |
| H  | 0         | 5.549075  | -1.059779 |
| H  | 2.01582   | -2.774538 | -4.489296 |
| H  | -5.277484 | -1.714759 | 1.059779  |
| H  | 3.261665  | 1.059779  | -4.489296 |
| H  | -3.261665 | -4.489296 | -1.059779 |
| H  | -3.261665 | 4.489296  | 1.059779  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.261665 | 1.059779  | -4.489296 |
| H | -2.01582  | -2.774538 | -4.489296 |
| H | -5.277484 | 1.714759  | -1.059779 |
| H | 0         | 3.429517  | -4.489296 |
| H | 5.277484  | 1.714759  | -1.059779 |
| H | 0         | -5.549075 | 1.059779  |
| H | -2.01582  | 2.774538  | 4.489296  |
| H | -3.261665 | -1.059779 | 4.489296  |
| H | 3.261665  | 4.489296  | 1.059779  |
| H | 3.261665  | -4.489296 | -1.059779 |
| H | 3.261665  | -1.059779 | 4.489296  |
| H | 0         | -3.429517 | 4.489296  |
| H | 2.01582   | 2.774538  | 4.489296  |
| H | 5.277484  | -1.714759 | 1.059779  |

Sn<sub>20</sub>H<sub>20</sub> ⊂ Ne

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ne | 0         | 0         | 0         |
| Sn | -2.269119 | -0.737281 | 3.123174  |
| Sn | 2.269119  | 3.123174  | 0.737281  |
| Sn | 2.269119  | -3.123174 | -0.737281 |
| Sn | 2.269119  | -0.737281 | 3.123174  |
| Sn | 0         | -3.860456 | 0.737281  |
| Sn | -1.402393 | 1.930228  | 3.123174  |
| Sn | 3.671511  | 1.192946  | -0.737281 |
| Sn | 0         | 3.860456  | -0.737281 |
| Sn | 1.402393  | -1.930228 | -3.123174 |
| Sn | -3.671511 | -1.192946 | 0.737281  |
| Sn | 2.269119  | 0.737281  | -3.123174 |
| Sn | -2.269119 | -3.123174 | -0.737281 |
| Sn | -2.269119 | 3.123174  | 0.737281  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | -2.269119 | 0.737281  | -3.123174 |
| Sn | -1.402393 | -1.930228 | -3.123174 |
| Sn | -3.671511 | 1.192946  | -0.737281 |
| Sn | 0         | 2.385893  | -3.123174 |
| Sn | 3.671511  | -1.192946 | 0.737281  |
| Sn | 0         | -2.385893 | 3.123174  |
| Sn | 1.402393  | 1.930228  | 3.123174  |
| H  | 0         | 5.547762  | -1.059528 |
| H  | 2.015343  | -2.773881 | -4.488234 |
| H  | -5.276236 | -1.714353 | 1.059528  |
| H  | 3.260893  | 1.059528  | -4.488234 |
| H  | -3.260893 | -4.488234 | -1.059528 |
| H  | -3.260893 | 4.488234  | 1.059528  |
| H  | -3.260893 | 1.059528  | -4.488234 |
| H  | -2.015343 | -2.773881 | -4.488234 |
| H  | -5.276236 | 1.714353  | -1.059528 |
| H  | 0         | 3.428706  | -4.488234 |
| H  | 5.276236  | 1.714353  | -1.059528 |
| H  | 0         | -5.547762 | 1.059528  |
| H  | -2.015343 | 2.773881  | 4.488234  |
| H  | -3.260893 | -1.059528 | 4.488234  |
| H  | 3.260893  | 4.488234  | 1.059528  |
| H  | 3.260893  | -4.488234 | -1.059528 |
| H  | 3.260893  | -1.059528 | 4.488234  |
| H  | 0         | -3.428706 | 4.488234  |
| H  | 2.015343  | 2.773881  | 4.488234  |
| H  | 5.276236  | -1.714353 | 1.059528  |

$\text{Sn}_{20}\text{H}_{20} \subset \text{Ar}$

|    |   |   |   |
|----|---|---|---|
| Ar | 0 | 0 | 0 |
|----|---|---|---|

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | -2.272993 | -0.73854  | 3.128506  |
| Sn | 2.272993  | 3.128506  | 0.73854   |
| Sn | 2.272993  | -3.128506 | -0.73854  |
| Sn | 2.272993  | -0.73854  | 3.128506  |
| Sn | 0         | -3.867047 | 0.73854   |
| Sn | -1.404787 | 1.933523  | 3.128506  |
| Sn | 3.67778   | 1.194983  | -0.73854  |
| Sn | 0         | 3.867047  | -0.73854  |
| Sn | 1.404787  | -1.933523 | -3.128506 |
| Sn | -3.67778  | -1.194983 | 0.73854   |
| Sn | 2.272993  | 0.73854   | -3.128506 |
| Sn | -2.272993 | -3.128506 | -0.73854  |
| Sn | -2.272993 | 3.128506  | 0.73854   |
| Sn | -2.272993 | 0.73854   | -3.128506 |
| Sn | -1.404787 | -1.933523 | -3.128506 |
| Sn | -3.67778  | 1.194983  | -0.73854  |
| Sn | 0         | 2.389966  | -3.128506 |
| Sn | 3.67778   | -1.194983 | 0.73854   |
| Sn | 0         | -2.389966 | 3.128506  |
| Sn | 1.404787  | 1.933523  | 3.128506  |
| H  | 0         | 5.554537  | -1.060822 |
| H  | 2.017804  | -2.777269 | -4.493715 |
| H  | -5.282679 | -1.716446 | 1.060822  |
| H  | 3.264875  | 1.060822  | -4.493715 |
| H  | -3.264875 | -4.493715 | -1.060822 |
| H  | -3.264875 | 4.493715  | 1.060822  |
| H  | -3.264875 | 1.060822  | -4.493715 |
| H  | -2.017804 | -2.777269 | -4.493715 |
| H  | -5.282679 | 1.716446  | -1.060822 |
| H  | 0         | 3.432893  | -4.493715 |
| H  | 5.282679  | 1.716446  | -1.060822 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0         | -5.554537 | 1.060822  |
| H | -2.017804 | 2.777269  | 4.493715  |
| H | -3.264875 | -1.060822 | 4.493715  |
| H | 3.264875  | 4.493715  | 1.060822  |
| H | 3.264875  | -4.493715 | -1.060822 |
| H | 3.264875  | -1.060822 | 4.493715  |
| H | 0         | -3.432893 | 4.493715  |
| H | 2.017804  | 2.777269  | 4.493715  |
| H | 5.282679  | -1.716446 | 1.060822  |

$\text{Sn}_{20}\text{H}_{20} \subset \text{Kr}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Kr | 0         | 0         | 0         |
| Sn | -2.276959 | -0.739829 | 3.133965  |
| Sn | 2.276959  | 3.133965  | 0.739829  |
| Sn | 2.276959  | -3.133965 | -0.739829 |
| Sn | 2.276959  | -0.739829 | 3.133965  |
| Sn | 0         | -3.873793 | 0.739829  |
| Sn | -1.407238 | 1.936897  | 3.133965  |
| Sn | 3.684196  | 1.197068  | -0.739829 |
| Sn | 0         | 3.873793  | -0.739829 |
| Sn | 1.407238  | -1.936897 | -3.133965 |
| Sn | -3.684196 | -1.197068 | 0.739829  |
| Sn | 2.276959  | 0.739829  | -3.133965 |
| Sn | -2.276959 | -3.133965 | -0.739829 |
| Sn | -2.276959 | 3.133965  | 0.739829  |
| Sn | -2.276959 | 0.739829  | -3.133965 |
| Sn | -1.407238 | -1.936897 | -3.133965 |
| Sn | -3.684196 | 1.197068  | -0.739829 |
| Sn | 0         | 2.394136  | -3.133965 |
| Sn | 3.684196  | -1.197068 | 0.739829  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | 0         | -2.394136 | 3.133965  |
| Sn | 1.407238  | 1.936897  | 3.133965  |
| H  | 0         | 5.561549  | -1.062161 |
| H  | 2.020351  | -2.780774 | -4.499387 |
| H  | -5.289347 | -1.718613 | 1.062161  |
| H  | 3.268996  | 1.062161  | -4.499387 |
| H  | -3.268996 | -4.499387 | -1.062161 |
| H  | -3.268996 | 4.499387  | 1.062161  |
| H  | -3.268996 | 1.062161  | -4.499387 |
| H  | -2.020351 | -2.780774 | -4.499387 |
| H  | -5.289347 | 1.718613  | -1.062161 |
| H  | 0         | 3.437226  | -4.499387 |
| H  | 5.289347  | 1.718613  | -1.062161 |
| H  | 0         | -5.561549 | 1.062161  |
| H  | -2.020351 | 2.780774  | 4.499387  |
| H  | -3.268996 | -1.062161 | 4.499387  |
| H  | 3.268996  | 4.499387  | 1.062161  |
| H  | 3.268996  | -4.499387 | -1.062161 |
| H  | 3.268996  | -1.062161 | 4.499387  |
| H  | 0         | -3.437226 | 4.499387  |
| H  | 2.020351  | 2.780774  | 4.499387  |
| H  | 5.289347  | -1.718613 | 1.062161  |

$\text{Sn}_{20}\text{H}_{20} \subset \text{Xe}$

|    |          |           |           |
|----|----------|-----------|-----------|
| Xe | 0        | 0         | 0         |
| Sn | -2.28302 | -0.741798 | 3.142308  |
| Sn | 2.28302  | 3.142308  | 0.741798  |
| Sn | 2.28302  | -3.142308 | -0.741798 |
| Sn | 2.28302  | -0.741798 | 3.142308  |
| Sn | 0        | -3.884106 | 0.741798  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sn | -1.410984 | 1.942053  | 3.142308  |
| Sn | 3.694004  | 1.200255  | -0.741798 |
| Sn | 0         | 3.884106  | -0.741798 |
| Sn | 1.410984  | -1.942053 | -3.142308 |
| Sn | -3.694004 | -1.200255 | 0.741798  |
| Sn | 2.28302   | 0.741798  | -3.142308 |
| Sn | -2.28302  | -3.142308 | -0.741798 |
| Sn | -2.28302  | 3.142308  | 0.741798  |
| Sn | -2.28302  | 0.741798  | -3.142308 |
| Sn | -1.410984 | -1.942053 | -3.142308 |
| Sn | -3.694004 | 1.200255  | -0.741798 |
| Sn | 0         | 2.40051   | -3.142308 |
| Sn | 3.694004  | -1.200255 | 0.741798  |
| Sn | 0         | -2.40051  | 3.142308  |
| Sn | 1.410984  | 1.942053  | 3.142308  |
| H  | 0         | 5.572413  | -1.064236 |
| H  | 2.024298  | -2.786207 | -4.508177 |
| H  | -5.29968  | -1.72197  | 1.064236  |
| H  | 3.275382  | 1.064236  | -4.508177 |
| H  | -3.275382 | -4.508177 | -1.064236 |
| H  | -3.275382 | 4.508177  | 1.064236  |
| H  | -3.275382 | 1.064236  | -4.508177 |
| H  | -2.024298 | -2.786207 | -4.508177 |
| H  | -5.29968  | 1.72197   | -1.064236 |
| H  | 0         | 3.443941  | -4.508177 |
| H  | 5.29968   | 1.72197   | -1.064236 |
| H  | 0         | -5.572413 | 1.064236  |
| H  | -2.024298 | 2.786207  | 4.508177  |
| H  | -3.275382 | -1.064236 | 4.508177  |
| H  | 3.275382  | 4.508177  | 1.064236  |
| H  | 3.275382  | -4.508177 | -1.064236 |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 3.275382 | -1.064236 | 4.508177 |
| H | 0        | -3.443941 | 4.508177 |
| H | 2.024298 | 2.786207  | 4.508177 |
| H | 5.29968  | -1.72197  | 1.064236 |

$\text{Sn}_{20}\text{H}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Sn | -2.285855 | -0.742719 | 3.14621   |
| Sn | 2.285855  | 3.14621   | 0.742719  |
| Sn | 2.285855  | -3.14621  | -0.742719 |
| Sn | 2.285855  | -0.742719 | 3.14621   |
| Sn | 0         | -3.888929 | 0.742719  |
| Sn | -1.412736 | 1.944465  | 3.14621   |
| Sn | 3.698591  | 1.201745  | -0.742719 |
| Sn | 0         | 3.888929  | -0.742719 |
| Sn | 1.412736  | -1.944465 | -3.14621  |
| Sn | -3.698591 | -1.201745 | 0.742719  |
| Sn | 2.285855  | 0.742719  | -3.14621  |
| Sn | -2.285855 | -3.14621  | -0.742719 |
| Sn | -2.285855 | 3.14621   | 0.742719  |
| Sn | -2.285855 | 0.742719  | -3.14621  |
| Sn | -1.412736 | -1.944465 | -3.14621  |
| Sn | -3.698591 | 1.201745  | -0.742719 |
| Sn | 0         | 2.40349   | -3.14621  |
| Sn | 3.698591  | -1.201745 | 0.742719  |
| Sn | 0         | -2.40349  | 3.14621   |
| Sn | 1.412736  | 1.944465  | 3.14621   |
| H  | 0         | 5.577538  | -1.065215 |
| H  | 2.026159  | -2.788769 | -4.512323 |
| H  | -5.304554 | -1.723554 | 1.065215  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.278395  | 1.065215  | -4.512323 |
| H | -3.278395 | -4.512323 | -1.065215 |
| H | -3.278395 | 4.512323  | 1.065215  |
| H | -3.278395 | 1.065215  | -4.512323 |
| H | -2.026159 | -2.788769 | -4.512323 |
| H | -5.304554 | 1.723554  | -1.065215 |
| H | 0         | 3.447108  | -4.512323 |
| H | 5.304554  | 1.723554  | -1.065215 |
| H | 0         | -5.577538 | 1.065215  |
| H | -2.026159 | 2.788769  | 4.512323  |
| H | -3.278395 | -1.065215 | 4.512323  |
| H | 3.278395  | 4.512323  | 1.065215  |
| H | 3.278395  | -4.512323 | -1.065215 |
| H | 3.278395  | -1.065215 | 4.512323  |
| H | 0         | -3.447108 | 4.512323  |
| H | 2.026159  | 2.788769  | 4.512323  |
| H | 5.304554  | -1.723554 | 1.065215  |

Pb<sub>20</sub>H<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pb | -2.37353  | -0.771207 | 3.266884  |
| Pb | 2.37353   | 3.266884  | 0.771207  |
| Pb | 2.37353   | -3.266884 | -0.771207 |
| Pb | 2.37353   | -0.771207 | 3.266884  |
| Pb | 0         | -4.038091 | 0.771207  |
| Pb | -1.466922 | 2.019045  | 3.266884  |
| Pb | 3.840453  | 1.247839  | -0.771207 |
| Pb | 0         | 4.038091  | -0.771207 |
| Pb | 1.466922  | -2.019045 | -3.266884 |
| Pb | -3.840453 | -1.247839 | 0.771207  |
| Pb | 2.37353   | 0.771207  | -3.266884 |
| Pb | -2.37353  | -3.266884 | -0.771207 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pb | -2.37353  | 3.266884  | 0.771207  |
| Pb | -2.37353  | 0.771207  | -3.266884 |
| Pb | -1.466922 | -2.019045 | -3.266884 |
| Pb | -3.840453 | 1.247839  | -0.771207 |
| Pb | 0         | 2.495677  | -3.266884 |
| Pb | 3.840453  | -1.247839 | 0.771207  |
| Pb | 0         | -2.495677 | 3.266884  |
| Pb | 1.466922  | 2.019045  | 3.266884  |
| H  | 0         | 5.788459  | -1.105497 |
| H  | 2.102781  | -2.894229 | -4.682962 |
| H  | -5.505152 | -1.788732 | 1.105497  |
| H  | 3.402371  | 1.105497  | -4.682962 |
| H  | -3.402371 | -4.682962 | -1.105497 |
| H  | -3.402371 | 4.682962  | 1.105497  |
| H  | -3.402371 | 1.105497  | -4.682962 |
| H  | -2.102781 | -2.894229 | -4.682962 |
| H  | -5.505152 | 1.788732  | -1.105497 |
| H  | 0         | 3.577464  | -4.682962 |
| H  | 5.505152  | 1.788732  | -1.105497 |
| H  | 0         | -5.788459 | 1.105497  |
| H  | -2.102781 | 2.894229  | 4.682962  |
| H  | -3.402371 | -1.105497 | 4.682962  |
| H  | 3.402371  | 4.682962  | 1.105497  |
| H  | 3.402371  | -4.682962 | -1.105497 |
| H  | 3.402371  | -1.105497 | 4.682962  |
| H  | 0         | -3.577464 | 4.682962  |
| H  | 2.102781  | 2.894229  | 4.682962  |
| H  | 5.505152  | -1.788732 | 1.105497  |

$\text{Pb}_{20}\text{H}_{20} \subset \text{He}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Pb | -2.373227 | -0.771108 | 3.266467  |
| Pb | 2.373227  | 3.266467  | 0.771108  |
| Pb | 2.373227  | -3.266467 | -0.771108 |
| Pb | 2.373227  | -0.771108 | 3.266467  |
| Pb | 0         | -4.037576 | 0.771108  |
| Pb | -1.466735 | 2.018788  | 3.266467  |
| Pb | 3.839963  | 1.247679  | -0.771108 |
| Pb | 0         | 4.037576  | -0.771108 |
| Pb | 1.466735  | -2.018788 | -3.266467 |
| Pb | -3.839963 | -1.247679 | 0.771108  |
| Pb | 2.373227  | 0.771108  | -3.266467 |
| Pb | -2.373227 | -3.266467 | -0.771108 |
| Pb | -2.373227 | 3.266467  | 0.771108  |
| Pb | -2.373227 | 0.771108  | -3.266467 |
| Pb | -1.466735 | -2.018788 | -3.266467 |
| Pb | -3.839963 | 1.247679  | -0.771108 |
| Pb | 0         | 2.495359  | -3.266467 |
| Pb | 3.839963  | -1.247679 | 0.771108  |
| Pb | 0         | -2.495359 | 3.266467  |
| Pb | 1.466735  | 2.018788  | 3.266467  |
| H  | 0         | 5.78868   | -1.105539 |
| H  | 2.102861  | -2.89434  | -4.68314  |
| H  | -5.505362 | -1.7888   | 1.105539  |
| H  | 3.402501  | 1.105539  | -4.68314  |
| H  | -3.402501 | -4.68314  | -1.105539 |
| H  | -3.402501 | 4.68314   | 1.105539  |
| H  | -3.402501 | 1.105539  | -4.68314  |
| H  | -2.102861 | -2.89434  | -4.68314  |
| H  | -5.505362 | 1.7888    | -1.105539 |
| H  | 0         | 3.577601  | -4.68314  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 5.505362  | 1.7888    | -1.105539 |
| H | 0         | -5.78868  | 1.105539  |
| H | -2.102861 | 2.89434   | 4.68314   |
| H | -3.402501 | -1.105539 | 4.68314   |
| H | 3.402501  | 4.68314   | 1.105539  |
| H | 3.402501  | -4.68314  | -1.105539 |
| H | 3.402501  | -1.105539 | 4.68314   |
| H | 0         | -3.577601 | 4.68314   |
| H | 2.102861  | 2.89434   | 4.68314   |
| H | 5.505362  | -1.7888   | 1.105539  |

$\text{Pb}_{20}\text{H}_{20} \subset \text{Ne}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ne | 0         | 0         | 0         |
| Pb | -2.372402 | -0.77084  | 3.265331  |
| Pb | 2.372402  | 3.265331  | 0.77084   |
| Pb | 2.372402  | -3.265331 | -0.77084  |
| Pb | 2.372402  | -0.77084  | 3.265331  |
| Pb | 0         | -4.036171 | 0.77084   |
| Pb | -1.466225 | 2.018086  | 3.265331  |
| Pb | 3.838627  | 1.247246  | -0.77084  |
| Pb | 0         | 4.036171  | -0.77084  |
| Pb | 1.466225  | -2.018086 | -3.265331 |
| Pb | -3.838627 | -1.247246 | 0.77084   |
| Pb | 2.372402  | 0.77084   | -3.265331 |
| Pb | -2.372402 | -3.265331 | -0.77084  |
| Pb | -2.372402 | 3.265331  | 0.77084   |
| Pb | -2.372402 | 0.77084   | -3.265331 |
| Pb | -1.466225 | -2.018086 | -3.265331 |
| Pb | -3.838627 | 1.247246  | -0.77084  |
| Pb | 0         | 2.494491  | -3.265331 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pb | 3.838627  | -1.247246 | 0.77084   |
| Pb | 0         | -2.494491 | 3.265331  |
| Pb | 1.466225  | 2.018086  | 3.265331  |
| H  | 0         | 5.787166  | -1.10525  |
| H  | 2.102311  | -2.893583 | -4.681916 |
| H  | -5.503922 | -1.788333 | 1.10525   |
| H  | 3.401611  | 1.10525   | -4.681916 |
| H  | -3.401611 | -4.681916 | -1.10525  |
| H  | -3.401611 | 4.681916  | 1.10525   |
| H  | -3.401611 | 1.10525   | -4.681916 |
| H  | -2.102311 | -2.893583 | -4.681916 |
| H  | -5.503922 | 1.788333  | -1.10525  |
| H  | 0         | 3.576666  | -4.681916 |
| H  | 5.503922  | 1.788333  | -1.10525  |
| H  | 0         | -5.787166 | 1.10525   |
| H  | -2.102311 | 2.893583  | 4.681916  |
| H  | -3.401611 | -1.10525  | 4.681916  |
| H  | 3.401611  | 4.681916  | 1.10525   |
| H  | 3.401611  | -4.681916 | -1.10525  |
| H  | 3.401611  | -1.10525  | 4.681916  |
| H  | 0         | -3.576666 | 4.681916  |
| H  | 2.102311  | 2.893583  | 4.681916  |
| H  | 5.503922  | -1.788333 | 1.10525   |

$\text{Pb}_{20}\text{H}_{20} \subset \text{Ar}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ar | 0         | 0         | 0         |
| Pb | -2.375612 | -0.771883 | 3.269749  |
| Pb | 2.375612  | 3.269749  | 0.771883  |
| Pb | 2.375612  | -3.269749 | -0.771883 |
| Pb | 2.375612  | -0.771883 | 3.269749  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pb | 0         | -4.041633 | 0.771883  |
| Pb | -1.468209 | 2.020816  | 3.269749  |
| Pb | 3.843821  | 1.248933  | -0.771883 |
| Pb | 0         | 4.041633  | -0.771883 |
| Pb | 1.468209  | -2.020816 | -3.269749 |
| Pb | -3.843821 | -1.248933 | 0.771883  |
| Pb | 2.375612  | 0.771883  | -3.269749 |
| Pb | -2.375612 | -3.269749 | -0.771883 |
| Pb | -2.375612 | 3.269749  | 0.771883  |
| Pb | -2.375612 | 0.771883  | -3.269749 |
| Pb | -1.468209 | -2.020816 | -3.269749 |
| Pb | -3.843821 | 1.248933  | -0.771883 |
| Pb | 0         | 2.497866  | -3.269749 |
| Pb | 3.843821  | -1.248933 | 0.771883  |
| Pb | 0         | -2.497866 | 3.269749  |
| Pb | 1.468209  | 2.020816  | 3.269749  |
| H  | 0         | 5.793188  | -1.1064   |
| H  | 2.104499  | -2.896594 | -4.686787 |
| H  | -5.509649 | -1.790193 | 1.1064    |
| H  | 3.40515   | 1.1064    | -4.686787 |
| H  | -3.40515  | -4.686787 | -1.1064   |
| H  | -3.40515  | 4.686787  | 1.1064    |
| H  | -3.40515  | 1.1064    | -4.686787 |
| H  | -2.104499 | -2.896594 | -4.686787 |
| H  | -5.509649 | 1.790193  | -1.1064   |
| H  | 0         | 3.580387  | -4.686787 |
| H  | 5.509649  | 1.790193  | -1.1064   |
| H  | 0         | -5.793188 | 1.1064    |
| H  | -2.104499 | 2.896594  | 4.686787  |
| H  | -3.40515  | -1.1064   | 4.686787  |
| H  | 3.40515   | 4.686787  | 1.1064    |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 3.40515  | -4.686787 | -1.1064  |
| H | 3.40515  | -1.1064   | 4.686787 |
| H | 0        | -3.580387 | 4.686787 |
| H | 2.104499 | 2.896594  | 4.686787 |
| H | 5.509649 | -1.790193 | 1.1064   |

Pb<sub>20</sub>H<sub>20</sub>  $\subset$  Kr

|    |           |           |           |
|----|-----------|-----------|-----------|
| Kr | 0         | 0         | 0         |
| Pb | -2.378474 | -0.772813 | 3.273688  |
| Pb | 2.378474  | 3.273688  | 0.772813  |
| Pb | 2.378474  | -3.273688 | -0.772813 |
| Pb | 2.378474  | -0.772813 | 3.273688  |
| Pb | 0         | -4.046501 | 0.772813  |
| Pb | -1.469978 | 2.023251  | 3.273688  |
| Pb | 3.848451  | 1.250438  | -0.772813 |
| Pb | 0         | 4.046501  | -0.772813 |
| Pb | 1.469978  | -2.023251 | -3.273688 |
| Pb | -3.848451 | -1.250438 | 0.772813  |
| Pb | 2.378474  | 0.772813  | -3.273688 |
| Pb | -2.378474 | -3.273688 | -0.772813 |
| Pb | -2.378474 | 3.273688  | 0.772813  |
| Pb | -2.378474 | 0.772813  | -3.273688 |
| Pb | -1.469978 | -2.023251 | -3.273688 |
| Pb | -3.848451 | 1.250438  | -0.772813 |
| Pb | 0         | 2.500875  | -3.273688 |
| Pb | 3.848451  | -1.250438 | 0.772813  |
| Pb | 0         | -2.500875 | 3.273688  |
| Pb | 1.469978  | 2.023251  | 3.273688  |
| H  | 0         | 5.797334  | -1.107192 |
| H  | 2.106005  | -2.898667 | -4.690142 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -5.513593 | -1.791475 | 1.107192  |
| H | 3.407588  | 1.107192  | -4.690142 |
| H | -3.407588 | -4.690142 | -1.107192 |
| H | -3.407588 | 4.690142  | 1.107192  |
| H | -3.407588 | 1.107192  | -4.690142 |
| H | -2.106005 | -2.898667 | -4.690142 |
| H | -5.513593 | 1.791475  | -1.107192 |
| H | 0         | 3.58295   | -4.690142 |
| H | 5.513593  | 1.791475  | -1.107192 |
| H | 0         | -5.797334 | 1.107192  |
| H | -2.106005 | 2.898667  | 4.690142  |
| H | -3.407588 | -1.107192 | 4.690142  |
| H | 3.407588  | 4.690142  | 1.107192  |
| H | 3.407588  | -4.690142 | -1.107192 |
| H | 3.407588  | -1.107192 | 4.690142  |
| H | 0         | -3.58295  | 4.690142  |
| H | 2.106005  | 2.898667  | 4.690142  |
| H | 5.513593  | -1.791475 | 1.107192  |

$\text{Pb}_{20}\text{H}_{20} \subset \text{Xe}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Xe | 0         | 0         | 0         |
| Pb | -2.385109 | -0.774969 | 3.282821  |
| Pb | 2.385109  | 3.282821  | 0.774969  |
| Pb | 2.385109  | -3.282821 | -0.774969 |
| Pb | 2.385109  | -0.774969 | 3.282821  |
| Pb | 0         | -4.05779  | 0.774969  |
| Pb | -1.474078 | 2.028895  | 3.282821  |
| Pb | 3.859187  | 1.253926  | -0.774969 |
| Pb | 0         | 4.05779   | -0.774969 |
| Pb | 1.474078  | -2.028895 | -3.282821 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pb | -3.859187 | -1.253926 | 0.774969  |
| Pb | 2.385109  | 0.774969  | -3.282821 |
| Pb | -2.385109 | -3.282821 | -0.774969 |
| Pb | -2.385109 | 3.282821  | 0.774969  |
| Pb | -2.385109 | 0.774969  | -3.282821 |
| Pb | -1.474078 | -2.028895 | -3.282821 |
| Pb | -3.859187 | 1.253926  | -0.774969 |
| Pb | 0         | 2.507852  | -3.282821 |
| Pb | 3.859187  | -1.253926 | 0.774969  |
| Pb | 0         | -2.507852 | 3.282821  |
| Pb | 1.474078  | 2.028895  | 3.282821  |
| H  | 0         | 5.809412  | -1.109499 |
| H  | 2.110393  | -2.904706 | -4.699913 |
| H  | -5.52508  | -1.795207 | 1.109499  |
| H  | 3.414687  | 1.109499  | -4.699913 |
| H  | -3.414687 | -4.699913 | -1.109499 |
| H  | -3.414687 | 4.699913  | 1.109499  |
| H  | -3.414687 | 1.109499  | -4.699913 |
| H  | -2.110393 | -2.904706 | -4.699913 |
| H  | -5.52508  | 1.795207  | -1.109499 |
| H  | 0         | 3.590414  | -4.699913 |
| H  | 5.52508   | 1.795207  | -1.109499 |
| H  | 0         | -5.809412 | 1.109499  |
| H  | -2.110393 | 2.904706  | 4.699913  |
| H  | -3.414687 | -1.109499 | 4.699913  |
| H  | 3.414687  | 4.699913  | 1.109499  |
| H  | 3.414687  | -4.699913 | -1.109499 |
| H  | 3.414687  | -1.109499 | 4.699913  |
| H  | 0         | -3.590414 | 4.699913  |
| H  | 2.110393  | 2.904706  | 4.699913  |
| H  | 5.52508   | -1.795207 | 1.109499  |

$\text{Pb}_{20}\text{H}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Pb | -2.388697 | -0.776135 | 3.28776   |
| Pb | 2.388697  | 3.28776   | 0.776135  |
| Pb | 2.388697  | -3.28776  | -0.776135 |
| Pb | 2.388697  | -0.776135 | 3.28776   |
| Pb | 0         | -4.063895 | 0.776135  |
| Pb | -1.476296 | 2.031947  | 3.28776   |
| Pb | 3.864994  | 1.255813  | -0.776135 |
| Pb | 0         | 4.063895  | -0.776135 |
| Pb | 1.476296  | -2.031947 | -3.28776  |
| Pb | -3.864994 | -1.255813 | 0.776135  |
| Pb | 2.388697  | 0.776135  | -3.28776  |
| Pb | -2.388697 | -3.28776  | -0.776135 |
| Pb | -2.388697 | 3.28776   | 0.776135  |
| Pb | -2.388697 | 0.776135  | -3.28776  |
| Pb | -1.476296 | -2.031947 | -3.28776  |
| Pb | -3.864994 | 1.255813  | -0.776135 |
| Pb | 0         | 2.511625  | -3.28776  |
| Pb | 3.864994  | -1.255813 | 0.776135  |
| Pb | 0         | -2.511625 | 3.28776   |
| Pb | 1.476296  | 2.031947  | 3.28776   |
| H  | 0         | 5.815973  | -1.110752 |
| H  | 2.112776  | -2.907987 | -4.705221 |
| H  | -5.531319 | -1.797235 | 1.110752  |
| H  | 3.418543  | 1.110752  | -4.705221 |
| H  | -3.418543 | -4.705221 | -1.110752 |
| H  | -3.418543 | 4.705221  | 1.110752  |
| H  | -3.418543 | 1.110752  | -4.705221 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.112776 | -2.907987 | -4.705221 |
| H | -5.531319 | 1.797235  | -1.110752 |
| H | 0         | 3.594469  | -4.705221 |
| H | 5.531319  | 1.797235  | -1.110752 |
| H | 0         | -5.815973 | 1.110752  |
| H | -2.112776 | 2.907987  | 4.705221  |
| H | -3.418543 | -1.110752 | 4.705221  |
| H | 3.418543  | 4.705221  | 1.110752  |
| H | 3.418543  | -4.705221 | -1.110752 |
| H | 3.418543  | -1.110752 | 4.705221  |
| H | 0         | -3.594469 | 4.705221  |
| H | 2.112776  | 2.907987  | 4.705221  |
| H | 5.531319  | -1.797235 | 1.110752  |

N<sub>20</sub>

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -1.192808 | -0.387567 | 1.641759  |
| N | 0         | -1.254192 | 1.641759  |
| N | 1.192808  | -0.387567 | 1.641759  |
| N | 0.737196  | 1.014663  | 1.641759  |
| N | -0.737196 | 1.014663  | 1.641759  |
| N | 0         | -2.029325 | 0.387567  |
| N | -1.192808 | -1.641759 | -0.387567 |
| N | -1.930003 | -0.627096 | 0.387567  |
| N | 1.192808  | -1.641759 | -0.387567 |
| N | 1.930003  | -0.627096 | 0.387567  |
| N | 1.930003  | 0.627096  | -0.387567 |
| N | 1.192808  | 1.641759  | 0.387567  |
| N | 0         | 2.029325  | -0.387567 |
| N | -1.192808 | 1.641759  | 0.387567  |
| N | -1.930003 | 0.627096  | -0.387567 |
| N | 0.737196  | -1.014663 | -1.641759 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | 1.192808  | 0.387567  | -1.641759 |
| N | 0         | 1.254192  | -1.641759 |
| N | -1.192808 | 0.387567  | -1.641759 |
| N | -0.737196 | -1.014663 | -1.641759 |

$N_{20} \subset He$

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | -1.192808 | -0.387567 | 1.641759  |
| N  | 0         | -1.254192 | 1.641759  |
| N  | 1.192808  | -0.387567 | 1.641759  |
| N  | 0.737196  | 1.014663  | 1.641759  |
| N  | -0.737196 | 1.014663  | 1.641759  |
| N  | 0         | -2.029325 | 0.387567  |
| N  | -1.192808 | -1.641759 | -0.387567 |
| N  | -1.930003 | -0.627096 | 0.387567  |
| N  | 1.192808  | -1.641759 | -0.387567 |
| N  | 1.930003  | -0.627096 | 0.387567  |
| N  | 1.930003  | 0.627096  | -0.387567 |
| N  | 1.192808  | 1.641759  | 0.387567  |
| N  | 0         | 2.029325  | -0.387567 |
| N  | -1.192808 | 1.641759  | 0.387567  |
| N  | -1.930003 | 0.627096  | -0.387567 |
| N  | 0.737196  | -1.014663 | -1.641759 |
| N  | 1.192808  | 0.387567  | -1.641759 |
| N  | 0         | 1.254192  | -1.641759 |
| N  | -1.192808 | 0.387567  | -1.641759 |
| N  | -0.737196 | -1.014663 | -1.641759 |
| He | 0         | 0         | 0         |

$N_{20} \subset Ne$

|   |           |           |          |
|---|-----------|-----------|----------|
| N | -1.215643 | -0.394986 | 1.673189 |
|---|-----------|-----------|----------|

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | 0         | -1.278203 | 1.673189  |
| N  | 1.215643  | -0.394986 | 1.673189  |
| N  | 0.751309  | 1.034088  | 1.673189  |
| N  | -0.751309 | 1.034088  | 1.673189  |
| N  | 0         | -2.068175 | 0.394986  |
| N  | -1.215643 | -1.673189 | -0.394986 |
| N  | -1.966952 | -0.639101 | 0.394986  |
| N  | 1.215643  | -1.673189 | -0.394986 |
| N  | 1.966952  | -0.639101 | 0.394986  |
| N  | 1.966952  | 0.639101  | -0.394986 |
| N  | 1.215643  | 1.673189  | 0.394986  |
| N  | 0         | 2.068175  | -0.394986 |
| N  | -1.215643 | 1.673189  | 0.394986  |
| N  | -1.966952 | 0.639101  | -0.394986 |
| N  | 0.751309  | -1.034088 | -1.673189 |
| N  | 1.215643  | 0.394986  | -1.673189 |
| N  | 0         | 1.278203  | -1.673189 |
| N  | -1.215643 | 0.394986  | -1.673189 |
| N  | -0.751309 | -1.034088 | -1.673189 |
| Ne | 0         | 0         | 0         |

$N_{20} \subset Ar$

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -1.274956 | -0.414258 | 1.754827  |
| N | 0         | -1.340568 | 1.754827  |
| N | 1.274956  | -0.414258 | 1.754827  |
| N | 0.787966  | 1.084543  | 1.754827  |
| N | -0.787966 | 1.084543  | 1.754827  |
| N | 0         | -2.169085 | 0.414258  |
| N | -1.274956 | -1.754827 | -0.414258 |
| N | -2.062923 | -0.670284 | 0.414258  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | 1.274956  | -1.754827 | -0.414258 |
| N  | 2.062923  | -0.670284 | 0.414258  |
| N  | 2.062923  | 0.670284  | -0.414258 |
| N  | 1.274956  | 1.754827  | 0.414258  |
| N  | 0         | 2.169085  | -0.414258 |
| N  | -1.274956 | 1.754827  | 0.414258  |
| N  | -2.062923 | 0.670284  | -0.414258 |
| N  | 0.787966  | -1.084543 | -1.754827 |
| N  | 1.274956  | 0.414258  | -1.754827 |
| N  | 0         | 1.340568  | -1.754827 |
| N  | -1.274956 | 0.414258  | -1.754827 |
| N  | -0.787966 | -1.084543 | -1.754827 |
| Ar | 0         | 0         | 0         |

$N_{20} \subset Kr$

|   |           |           |           |
|---|-----------|-----------|-----------|
| N | -1.310337 | -0.425754 | 1.803524  |
| N | 0         | -1.37777  | 1.803524  |
| N | 1.310337  | -0.425754 | 1.803524  |
| N | 0.809833  | 1.114639  | 1.803524  |
| N | -0.809833 | 1.114639  | 1.803524  |
| N | 0         | -2.229278 | 0.425754  |
| N | -1.310337 | -1.803524 | -0.425754 |
| N | -2.12017  | -0.688885 | 0.425754  |
| N | 1.310337  | -1.803524 | -0.425754 |
| N | 2.12017   | -0.688885 | 0.425754  |
| N | 2.12017   | 0.688885  | -0.425754 |
| N | 1.310337  | 1.803524  | 0.425754  |
| N | 0         | 2.229278  | -0.425754 |
| N | -1.310337 | 1.803524  | 0.425754  |
| N | -2.12017  | 0.688885  | -0.425754 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | 0.809833  | -1.114639 | -1.803524 |
| N  | 1.310337  | 0.425754  | -1.803524 |
| N  | 0         | 1.37777   | -1.803524 |
| N  | -1.310337 | 0.425754  | -1.803524 |
| N  | -0.809833 | -1.114639 | -1.803524 |
| Kr | 0         | 0         | 0         |

$N_{20} \subset Xe$

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | -1.346024 | -0.43735  | 1.852644  |
| N  | 0         | -1.415294 | 1.852644  |
| N  | 1.346024  | -0.43735  | 1.852644  |
| N  | 0.831889  | 1.144997  | 1.852644  |
| N  | -0.831889 | 1.144997  | 1.852644  |
| N  | 0         | -2.289994 | 0.43735   |
| N  | -1.346024 | -1.852644 | -0.43735  |
| N  | -2.177913 | -0.707647 | 0.43735   |
| N  | 1.346024  | -1.852644 | -0.43735  |
| N  | 2.177913  | -0.707647 | 0.43735   |
| N  | 2.177913  | 0.707647  | -0.43735  |
| N  | 1.346024  | 1.852644  | 0.43735   |
| N  | 0         | 2.289994  | -0.43735  |
| N  | -1.346024 | 1.852644  | 0.43735   |
| N  | -2.177913 | 0.707647  | -0.43735  |
| N  | 0.831889  | -1.144997 | -1.852644 |
| N  | 1.346024  | 0.43735   | -1.852644 |
| N  | 0         | 1.415294  | -1.852644 |
| N  | -1.346024 | 0.43735   | -1.852644 |
| N  | -0.831889 | -1.144997 | -1.852644 |
| Xe | 0         | 0         | 0         |

$N_{20} \subset R_n$

|    |           |           |           |
|----|-----------|-----------|-----------|
| N  | -1.358866 | -0.441522 | 1.870318  |
| N  | 0         | -1.428796 | 1.870318  |
| N  | 1.358866  | -0.441522 | 1.870318  |
| N  | 0.839825  | 1.15592   | 1.870318  |
| N  | -0.839825 | 1.15592   | 1.870318  |
| N  | 0         | -2.31184  | 0.441522  |
| N  | -1.358866 | -1.870318 | -0.441522 |
| N  | -2.198691 | -0.714398 | 0.441522  |
| N  | 1.358866  | -1.870318 | -0.441522 |
| N  | 2.198691  | -0.714398 | 0.441522  |
| N  | 2.198691  | 0.714398  | -0.441522 |
| N  | 1.358866  | 1.870318  | 0.441522  |
| N  | 0         | 2.31184   | -0.441522 |
| N  | -1.358866 | 1.870318  | 0.441522  |
| N  | -2.198691 | 0.714398  | -0.441522 |
| N  | 0.839825  | -1.15592  | -1.870318 |
| N  | 1.358866  | 0.441522  | -1.870318 |
| N  | 0         | 1.428796  | -1.870318 |
| N  | -1.358866 | 0.441522  | -1.870318 |
| N  | -0.839825 | -1.15592  | -1.870318 |
| Rn | 0         | 0         | 0         |

$P_{20}$

|   |           |           |          |
|---|-----------|-----------|----------|
| P | -1.823965 | -0.592642 | 2.510472 |
| P | 0         | -1.91783  | 2.510472 |
| P | 1.823965  | -0.592642 | 2.510472 |
| P | 1.127272  | 1.551557  | 2.510472 |
| P | -1.127272 | 1.551557  | 2.510472 |
| P | 0         | -3.103114 | 0.592642 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | -1.823965 | -2.510472 | -0.592642 |
| P | -2.951237 | -0.958915 | 0.592642  |
| P | 1.823965  | -2.510472 | -0.592642 |
| P | 2.951237  | -0.958915 | 0.592642  |
| P | 2.951237  | 0.958915  | -0.592642 |
| P | 1.823965  | 2.510472  | 0.592642  |
| P | 0         | 3.103114  | -0.592642 |
| P | -1.823965 | 2.510472  | 0.592642  |
| P | -2.951237 | 0.958915  | -0.592642 |
| P | 1.127272  | -1.551557 | -2.510472 |
| P | 1.823965  | 0.592642  | -2.510472 |
| P | 0         | 1.91783   | -2.510472 |
| P | -1.823965 | 0.592642  | -2.510472 |
| P | -1.127272 | -1.551557 | -2.510472 |

$P_{20} \subset \text{He}$

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | -1.826071 | -0.593327 | 2.513372  |
| P | 0         | -1.920045 | 2.513372  |
| P | 1.826071  | -0.593327 | 2.513372  |
| P | 1.128574  | 1.553349  | 2.513372  |
| P | -1.128574 | 1.553349  | 2.513372  |
| P | 0         | -3.106698 | 0.593327  |
| P | -1.826071 | -2.513372 | -0.593327 |
| P | -2.954646 | -0.960023 | 0.593327  |
| P | 1.826071  | -2.513372 | -0.593327 |
| P | 2.954646  | -0.960023 | 0.593327  |
| P | 2.954646  | 0.960023  | -0.593327 |
| P | 1.826071  | 2.513372  | 0.593327  |
| P | 0         | 3.106698  | -0.593327 |
| P | -1.826071 | 2.513372  | 0.593327  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -2.954646 | 0.960023  | -0.593327 |
| P  | 1.128574  | -1.553349 | -2.513372 |
| P  | 1.826071  | 0.593327  | -2.513372 |
| P  | 0         | 1.920045  | -2.513372 |
| P  | -1.826071 | 0.593327  | -2.513372 |
| P  | -1.128574 | -1.553349 | -2.513372 |
| He | 0         | 0         | 0         |

$P_{20} \subset \text{Ne}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -1.828203 | -0.594019 | 2.516306  |
| P  | 0         | -1.922287 | 2.516306  |
| P  | 1.828203  | -0.594019 | 2.516306  |
| P  | 1.129892  | 1.555163  | 2.516306  |
| P  | -1.129892 | 1.555163  | 2.516306  |
| P  | 0         | -3.110325 | 0.594019  |
| P  | -1.828203 | -2.516306 | -0.594019 |
| P  | -2.958095 | -0.961143 | 0.594019  |
| P  | 1.828203  | -2.516306 | -0.594019 |
| P  | 2.958095  | -0.961143 | 0.594019  |
| P  | 2.958095  | 0.961143  | -0.594019 |
| P  | 1.828203  | 2.516306  | 0.594019  |
| P  | 0         | 3.110325  | -0.594019 |
| P  | -1.828203 | 2.516306  | 0.594019  |
| P  | -2.958095 | 0.961143  | -0.594019 |
| P  | 1.129892  | -1.555163 | -2.516306 |
| P  | 1.828203  | 0.594019  | -2.516306 |
| P  | 0         | 1.922287  | -2.516306 |
| P  | -1.828203 | 0.594019  | -2.516306 |
| P  | -1.129892 | -1.555163 | -2.516306 |
| Ne | 0         | 0         | 0         |

$P_{20} \subset Ar$

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -1.843011 | -0.598831 | 2.536687  |
| P  | 0         | -1.937856 | 2.536687  |
| P  | 1.843011  | -0.598831 | 2.536687  |
| P  | 1.139043  | 1.567759  | 2.536687  |
| P  | -1.139043 | 1.567759  | 2.536687  |
| P  | 0         | -3.135518 | 0.598831  |
| P  | -1.843011 | -2.536687 | -0.598831 |
| P  | -2.982054 | -0.968928 | 0.598831  |
| P  | 1.843011  | -2.536687 | -0.598831 |
| P  | 2.982054  | -0.968928 | 0.598831  |
| P  | 2.982054  | 0.968928  | -0.598831 |
| P  | 1.843011  | 2.536687  | 0.598831  |
| P  | 0         | 3.135518  | -0.598831 |
| P  | -1.843011 | 2.536687  | 0.598831  |
| P  | -2.982054 | 0.968928  | -0.598831 |
| P  | 1.139043  | -1.567759 | -2.536687 |
| P  | 1.843011  | 0.598831  | -2.536687 |
| P  | 0         | 1.937856  | -2.536687 |
| P  | -1.843011 | 0.598831  | -2.536687 |
| P  | -1.139043 | -1.567759 | -2.536687 |
| Ar | 0         | 0         | 0         |

$P_{20} \subset Kr$

|   |           |           |          |
|---|-----------|-----------|----------|
| P | -1.851851 | -0.601703 | 2.548854 |
| P | 0         | -1.947151 | 2.548854 |
| P | 1.851851  | -0.601703 | 2.548854 |
| P | 1.144507  | 1.575278  | 2.548854 |
| P | -1.144507 | 1.575278  | 2.548854 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | 0         | -3.150557 | 0.601703  |
| P  | -1.851851 | -2.548854 | -0.601703 |
| P  | -2.996358 | -0.973576 | 0.601703  |
| P  | 1.851851  | -2.548854 | -0.601703 |
| P  | 2.996358  | -0.973576 | 0.601703  |
| P  | 2.996358  | 0.973576  | -0.601703 |
| P  | 1.851851  | 2.548854  | 0.601703  |
| P  | 0         | 3.150557  | -0.601703 |
| P  | -1.851851 | 2.548854  | 0.601703  |
| P  | -2.996358 | 0.973576  | -0.601703 |
| P  | 1.144507  | -1.575278 | -2.548854 |
| P  | 1.851851  | 0.601703  | -2.548854 |
| P  | 0         | 1.947151  | -2.548854 |
| P  | -1.851851 | 0.601703  | -2.548854 |
| P  | -1.144507 | -1.575278 | -2.548854 |
| Kr | 0         | 0         | 0         |

$P_{20} \subset Xe$

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | -1.866872 | -0.606583 | 2.569529  |
| P | 0         | -1.962945 | 2.569529  |
| P | 1.866872  | -0.606583 | 2.569529  |
| P | 1.15379   | 1.588056  | 2.569529  |
| P | -1.15379  | 1.588056  | 2.569529  |
| P | 0         | -3.176112 | 0.606583  |
| P | -1.866872 | -2.569529 | -0.606583 |
| P | -3.020662 | -0.981473 | 0.606583  |
| P | 1.866872  | -2.569529 | -0.606583 |
| P | 3.020662  | -0.981473 | 0.606583  |
| P | 3.020662  | 0.981473  | -0.606583 |
| P | 1.866872  | 2.569529  | 0.606583  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | 0         | 3.176112  | -0.606583 |
| P  | -1.866872 | 2.569529  | 0.606583  |
| P  | -3.020662 | 0.981473  | -0.606583 |
| P  | 1.15379   | -1.588056 | -2.569529 |
| P  | 1.866872  | 0.606583  | -2.569529 |
| P  | 0         | 1.962945  | -2.569529 |
| P  | -1.866872 | 0.606583  | -2.569529 |
| P  | -1.15379  | -1.588056 | -2.569529 |
| Xe | 0         | 0         | 0         |

$P_{20} \subset R_n$

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | -1.875667 | -0.609441 | 2.581635  |
| P | 0         | -1.972193 | 2.581635  |
| P | 1.875667  | -0.609441 | 2.581635  |
| P | 1.159226  | 1.595538  | 2.581635  |
| P | -1.159226 | 1.595538  | 2.581635  |
| P | 0         | -3.191076 | 0.609441  |
| P | -1.875667 | -2.581635 | -0.609441 |
| P | -3.034894 | -0.986097 | 0.609441  |
| P | 1.875667  | -2.581635 | -0.609441 |
| P | 3.034894  | -0.986097 | 0.609441  |
| P | 3.034894  | 0.986097  | -0.609441 |
| P | 1.875667  | 2.581635  | 0.609441  |
| P | 0         | 3.191076  | -0.609441 |
| P | -1.875667 | 2.581635  | 0.609441  |
| P | -3.034894 | 0.986097  | -0.609441 |
| P | 1.159226  | -1.595538 | -2.581635 |
| P | 1.875667  | 0.609441  | -2.581635 |
| P | 0         | 1.972193  | -2.581635 |
| P | -1.875667 | 0.609441  | -2.581635 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -1.159226 | -1.595538 | -2.581635 |
| Rn | 0         | 0         | 0         |

As<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | -1.987006 | -0.645617 | 2.734879  |
| As | 0         | -2.089262 | 2.734879  |
| As | 1.987006  | -0.645617 | 2.734879  |
| As | 1.228037  | 1.690248  | 2.734879  |
| As | -1.228037 | 1.690248  | 2.734879  |
| As | 0         | -3.380496 | 0.645617  |
| As | -1.987006 | -2.734879 | -0.645617 |
| As | -3.215043 | -1.044631 | 0.645617  |
| As | 1.987006  | -2.734879 | -0.645617 |
| As | 3.215043  | -1.044631 | 0.645617  |
| As | 3.215043  | 1.044631  | -0.645617 |
| As | 1.987006  | 2.734879  | 0.645617  |
| As | 0         | 3.380496  | -0.645617 |
| As | -1.987006 | 2.734879  | 0.645617  |
| As | -3.215043 | 1.044631  | -0.645617 |
| As | 1.228037  | -1.690248 | -2.734879 |
| As | 1.987006  | 0.645617  | -2.734879 |
| As | 0         | 2.089262  | -2.734879 |
| As | -1.987006 | 0.645617  | -2.734879 |
| As | -1.228037 | -1.690248 | -2.734879 |

As<sub>20</sub> ⊂ He

|    |           |           |          |
|----|-----------|-----------|----------|
| As | -1.987855 | -0.645893 | 2.736047 |
| As | 0         | -2.090154 | 2.736047 |
| As | 1.987855  | -0.645893 | 2.736047 |
| As | 1.228562  | 1.69097   | 2.736047 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | -1.228562 | 1.69097   | 2.736047  |
| As | 0         | -3.38194  | 0.645893  |
| As | -1.987855 | -2.736047 | -0.645893 |
| As | -3.216416 | -1.045077 | 0.645893  |
| As | 1.987855  | -2.736047 | -0.645893 |
| As | 3.216416  | -1.045077 | 0.645893  |
| As | 3.216416  | 1.045077  | -0.645893 |
| As | 1.987855  | 2.736047  | 0.645893  |
| As | 0         | 3.38194   | -0.645893 |
| As | -1.987855 | 2.736047  | 0.645893  |
| As | -3.216416 | 1.045077  | -0.645893 |
| As | 1.228562  | -1.69097  | -2.736047 |
| As | 1.987855  | 0.645893  | -2.736047 |
| As | 0         | 2.090154  | -2.736047 |
| As | -1.987855 | 0.645893  | -2.736047 |
| As | -1.228562 | -1.69097  | -2.736047 |
| He | 0         | 0         | 0         |

As<sub>20</sub>  $\subset$  Ne

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | -1.989434 | -0.646406 | 2.738222  |
| As | 0         | -2.091815 | 2.738222  |
| As | 1.989434  | -0.646406 | 2.738222  |
| As | 1.229538  | 1.692314  | 2.738222  |
| As | -1.229538 | 1.692314  | 2.738222  |
| As | 0         | -3.384628 | 0.646406  |
| As | -1.989434 | -2.738222 | -0.646406 |
| As | -3.218973 | -1.045908 | 0.646406  |
| As | 1.989434  | -2.738222 | -0.646406 |
| As | 3.218973  | -1.045908 | 0.646406  |
| As | 3.218973  | 1.045908  | -0.646406 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | 1.989434  | 2.738222  | 0.646406  |
| As | 0         | 3.384628  | -0.646406 |
| As | -1.989434 | 2.738222  | 0.646406  |
| As | -3.218973 | 1.045908  | -0.646406 |
| As | 1.229538  | -1.692314 | -2.738222 |
| As | 1.989434  | 0.646406  | -2.738222 |
| As | 0         | 2.091815  | -2.738222 |
| As | -1.989434 | 0.646406  | -2.738222 |
| As | -1.229538 | -1.692314 | -2.738222 |
| Ne | 0         | 0         | 0         |

As<sub>20</sub>  $\subset$  Ar

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | -1.998763 | -0.649438 | 2.751062  |
| As | 0         | -2.101624 | 2.751062  |
| As | 1.998763  | -0.649438 | 2.751062  |
| As | 1.235304  | 1.70025   | 2.751062  |
| As | -1.235304 | 1.70025   | 2.751062  |
| As | 0         | -3.400499 | 0.649438  |
| As | -1.998763 | -2.751062 | -0.649438 |
| As | -3.234067 | -1.050812 | 0.649438  |
| As | 1.998763  | -2.751062 | -0.649438 |
| As | 3.234067  | -1.050812 | 0.649438  |
| As | 3.234067  | 1.050812  | -0.649438 |
| As | 1.998763  | 2.751062  | 0.649438  |
| As | 0         | 3.400499  | -0.649438 |
| As | -1.998763 | 2.751062  | 0.649438  |
| As | -3.234067 | 1.050812  | -0.649438 |
| As | 1.235304  | -1.70025  | -2.751062 |
| As | 1.998763  | 0.649438  | -2.751062 |
| As | 0         | 2.101624  | -2.751062 |

|    |           |          |           |
|----|-----------|----------|-----------|
| As | -1.998763 | 0.649438 | -2.751062 |
| As | -1.235304 | -1.70025 | -2.751062 |
| Ar | 0         | 0        | 0         |

As<sub>20</sub> ⊂ Kr

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | -2.006346 | -0.651901 | 2.761498  |
| As | 0         | -2.109597 | 2.761498  |
| As | 2.006346  | -0.651901 | 2.761498  |
| As | 1.23999   | 1.7067    | 2.761498  |
| As | -1.23999  | 1.7067    | 2.761498  |
| As | 0         | -3.413399 | 0.651901  |
| As | -2.006346 | -2.761498 | -0.651901 |
| As | -3.246336 | -1.054798 | 0.651901  |
| As | 2.006346  | -2.761498 | -0.651901 |
| As | 3.246336  | -1.054798 | 0.651901  |
| As | 3.246336  | 1.054798  | -0.651901 |
| As | 2.006346  | 2.761498  | 0.651901  |
| As | 0         | 3.413399  | -0.651901 |
| As | -2.006346 | 2.761498  | 0.651901  |
| As | -3.246336 | 1.054798  | -0.651901 |
| As | 1.23999   | -1.7067   | -2.761498 |
| As | 2.006346  | 0.651901  | -2.761498 |
| As | 0         | 2.109597  | -2.761498 |
| As | -2.006346 | 0.651901  | -2.761498 |
| As | -1.23999  | -1.7067   | -2.761498 |
| Kr | 0         | 0         | 0         |

As<sub>20</sub> ⊂ Xe

|    |           |           |          |
|----|-----------|-----------|----------|
| As | -2.018344 | -0.6558   | 2.778013 |
| As | 0         | -2.122213 | 2.778013 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | 2.018344  | -0.6558   | 2.778013  |
| As | 1.247405  | 1.716906  | 2.778013  |
| As | -1.247405 | 1.716906  | 2.778013  |
| As | 0         | -3.433813 | 0.6558    |
| As | -2.018344 | -2.778013 | -0.6558   |
| As | -3.26575  | -1.061106 | 0.6558    |
| As | 2.018344  | -2.778013 | -0.6558   |
| As | 3.26575   | -1.061106 | 0.6558    |
| As | 3.26575   | 1.061106  | -0.6558   |
| As | 2.018344  | 2.778013  | 0.6558    |
| As | 0         | 3.433813  | -0.6558   |
| As | -2.018344 | 2.778013  | 0.6558    |
| As | -3.26575  | 1.061106  | -0.6558   |
| As | 1.247405  | -1.716906 | -2.778013 |
| As | 2.018344  | 0.6558    | -2.778013 |
| As | 0         | 2.122213  | -2.778013 |
| As | -2.018344 | 0.6558    | -2.778013 |
| As | -1.247405 | -1.716906 | -2.778013 |
| Xe | 0         | 0         | 0         |

$\text{As}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| As | -2.025654 | -0.658175 | 2.788073  |
| As | 0         | -2.129898 | 2.788073  |
| As | 2.025654  | -0.658175 | 2.788073  |
| As | 1.251923  | 1.723124  | 2.788073  |
| As | -1.251923 | 1.723124  | 2.788073  |
| As | 0         | -3.446248 | 0.658175  |
| As | -2.025654 | -2.788073 | -0.658175 |
| As | -3.277577 | -1.064949 | 0.658175  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| As | 2.025654  | -2.788073 | -0.658175 |
| As | 3.277577  | -1.064949 | 0.658175  |
| As | 3.277577  | 1.064949  | -0.658175 |
| As | 2.025654  | 2.788073  | 0.658175  |
| As | 0         | 3.446248  | -0.658175 |
| As | -2.025654 | 2.788073  | 0.658175  |
| As | -3.277577 | 1.064949  | -0.658175 |
| As | 1.251923  | -1.723124 | -2.788073 |
| As | 2.025654  | 0.658175  | -2.788073 |
| As | 0         | 2.129898  | -2.788073 |
| As | -2.025654 | 0.658175  | -2.788073 |
| As | -1.251923 | -1.723124 | -2.788073 |

Sb<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sb | -2.296637 | -0.746223 | 3.16105   |
| Sb | 0         | -2.414827 | 3.16105   |
| Sb | 2.296637  | -0.746223 | 3.16105   |
| Sb | 1.4194    | 1.953636  | 3.16105   |
| Sb | -1.4194   | 1.953636  | 3.16105   |
| Sb | 0         | -3.907273 | 0.746223  |
| Sb | -2.296637 | -3.16105  | -0.746223 |
| Sb | -3.716037 | -1.207414 | 0.746223  |
| Sb | 2.296637  | -3.16105  | -0.746223 |
| Sb | 3.716037  | -1.207414 | 0.746223  |
| Sb | 3.716037  | 1.207414  | -0.746223 |
| Sb | 2.296637  | 3.16105   | 0.746223  |
| Sb | 0         | 3.907273  | -0.746223 |
| Sb | -2.296637 | 3.16105   | 0.746223  |
| Sb | -3.716037 | 1.207414  | -0.746223 |
| Sb | 1.4194    | -1.953636 | -3.16105  |
| Sb | 2.296637  | 0.746223  | -3.16105  |

|    |           |           |          |
|----|-----------|-----------|----------|
| Sb | 0         | 2.414827  | -3.16105 |
| Sb | -2.296637 | 0.746223  | -3.16105 |
| Sb | -1.4194   | -1.953636 | -3.16105 |

Sb<sub>20</sub>  $\subset$  He

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Sb | -2.296638 | -0.746223 | 3.16105   |
| Sb | 0         | -2.414828 | 3.16105   |
| Sb | 2.296638  | -0.746223 | 3.16105   |
| Sb | 1.4194    | 1.953637  | 3.16105   |
| Sb | -1.4194   | 1.953637  | 3.16105   |
| Sb | 0         | -3.907273 | 0.746223  |
| Sb | -2.296638 | -3.16105  | -0.746223 |
| Sb | -3.716038 | -1.207414 | 0.746223  |
| Sb | 2.296638  | -3.16105  | -0.746223 |
| Sb | 3.716038  | -1.207414 | 0.746223  |
| Sb | 3.716038  | 1.207414  | -0.746223 |
| Sb | 2.296638  | 3.16105   | 0.746223  |
| Sb | 0         | 3.907273  | -0.746223 |
| Sb | -2.296638 | 3.16105   | 0.746223  |
| Sb | -3.716038 | 1.207414  | -0.746223 |
| Sb | 1.4194    | -1.953637 | -3.16105  |
| Sb | 2.296638  | 0.746223  | -3.16105  |
| Sb | 0         | 2.414828  | -3.16105  |
| Sb | -2.296638 | 0.746223  | -3.16105  |
| Sb | -1.4194   | -1.953637 | -3.16105  |

Sb<sub>20</sub>  $\subset$  Ne

|    |           |           |         |
|----|-----------|-----------|---------|
| Ne | 0         | 0         | 0       |
| Sb | -2.296638 | -0.746223 | 3.16105 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sb | 0         | -2.414828 | 3.16105   |
| Sb | 2.296638  | -0.746223 | 3.16105   |
| Sb | 1.4194    | 1.953637  | 3.16105   |
| Sb | -1.4194   | 1.953637  | 3.16105   |
| Sb | 0         | -3.907273 | 0.746223  |
| Sb | -2.296638 | -3.16105  | -0.746223 |
| Sb | -3.716038 | -1.207414 | 0.746223  |
| Sb | 2.296638  | -3.16105  | -0.746223 |
| Sb | 3.716038  | -1.207414 | 0.746223  |
| Sb | 3.716038  | 1.207414  | -0.746223 |
| Sb | 2.296638  | 3.16105   | 0.746223  |
| Sb | 0         | 3.907273  | -0.746223 |
| Sb | -2.296638 | 3.16105   | 0.746223  |
| Sb | -3.716038 | 1.207414  | -0.746223 |
| Sb | 1.4194    | -1.953637 | -3.16105  |
| Sb | 2.296638  | 0.746223  | -3.16105  |
| Sb | 0         | 2.414828  | -3.16105  |
| Sb | -2.296638 | 0.746223  | -3.16105  |
| Sb | -1.4194   | -1.953637 | -3.16105  |

Sb<sub>20</sub>  $\subset$  Ar

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ar | 0         | 0         | 0         |
| Sb | -2.301249 | -0.747721 | 3.167397  |
| Sb | 0         | -2.419676 | 3.167397  |
| Sb | 2.301249  | -0.747721 | 3.167397  |
| Sb | 1.42225   | 1.957559  | 3.167397  |
| Sb | -1.42225  | 1.957559  | 3.167397  |
| Sb | 0         | -3.915118 | 0.747721  |
| Sb | -2.301249 | -3.167397 | -0.747721 |
| Sb | -3.723499 | -1.209838 | 0.747721  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sb | 2.301249  | -3.167397 | -0.747721 |
| Sb | 3.723499  | -1.209838 | 0.747721  |
| Sb | 3.723499  | 1.209838  | -0.747721 |
| Sb | 2.301249  | 3.167397  | 0.747721  |
| Sb | 0         | 3.915118  | -0.747721 |
| Sb | -2.301249 | 3.167397  | 0.747721  |
| Sb | -3.723499 | 1.209838  | -0.747721 |
| Sb | 1.42225   | -1.957559 | -3.167397 |
| Sb | 2.301249  | 0.747721  | -3.167397 |
| Sb | 0         | 2.419676  | -3.167397 |
| Sb | -2.301249 | 0.747721  | -3.167397 |
| Sb | -1.42225  | -1.957559 | -3.167397 |

$\text{Sb}_{20} \subset \text{Kr}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Kr | 0         | 0         | 0         |
| Sb | -2.30532  | -0.749044 | 3.173001  |
| Sb | 0         | -2.423957 | 3.173001  |
| Sb | 2.30532   | -0.749044 | 3.173001  |
| Sb | 1.424766  | 1.961022  | 3.173001  |
| Sb | -1.424766 | 1.961022  | 3.173001  |
| Sb | 0         | -3.922045 | 0.749044  |
| Sb | -2.30532  | -3.173001 | -0.749044 |
| Sb | -3.730086 | -1.211979 | 0.749044  |
| Sb | 2.30532   | -3.173001 | -0.749044 |
| Sb | 3.730086  | -1.211979 | 0.749044  |
| Sb | 3.730086  | 1.211979  | -0.749044 |
| Sb | 2.30532   | 3.173001  | 0.749044  |
| Sb | 0         | 3.922045  | -0.749044 |
| Sb | -2.30532  | 3.173001  | 0.749044  |
| Sb | -3.730086 | 1.211979  | -0.749044 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Sb | 1.424766  | -1.961022 | -3.173001 |
| Sb | 2.30532   | 0.749044  | -3.173001 |
| Sb | 0         | 2.423957  | -3.173001 |
| Sb | -2.30532  | 0.749044  | -3.173001 |
| Sb | -1.424766 | -1.961022 | -3.173001 |

$\text{Sb}_{20} \subset \text{Xe}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Xe | 0         | 0         | 0         |
| Sb | -2.312611 | -0.751413 | 3.183036  |
| Sb | 0         | -2.431623 | 3.183036  |
| Sb | 2.312611  | -0.751413 | 3.183036  |
| Sb | 1.429272  | 1.967224  | 3.183036  |
| Sb | -1.429272 | 1.967224  | 3.183036  |
| Sb | 0         | -3.934449 | 0.751413  |
| Sb | -2.312611 | -3.183036 | -0.751413 |
| Sb | -3.741883 | -1.215812 | 0.751413  |
| Sb | 2.312611  | -3.183036 | -0.751413 |
| Sb | 3.741883  | -1.215812 | 0.751413  |
| Sb | 3.741883  | 1.215812  | -0.751413 |
| Sb | 2.312611  | 3.183036  | 0.751413  |
| Sb | 0         | 3.934449  | -0.751413 |
| Sb | -2.312611 | 3.183036  | 0.751413  |
| Sb | -3.741883 | 1.215812  | -0.751413 |
| Sb | 1.429272  | -1.967224 | -3.183036 |
| Sb | 2.312611  | 0.751413  | -3.183036 |
| Sb | 0         | 2.431623  | -3.183036 |
| Sb | -2.312611 | 0.751413  | -3.183036 |
| Sb | -1.429272 | -1.967224 | -3.183036 |

$\text{Sb}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Sb | -2.315974 | -0.752505 | 3.187664  |
| Sb | 0         | -2.435159 | 3.187664  |
| Sb | 2.315974  | -0.752505 | 3.187664  |
| Sb | 1.43135   | 1.970085  | 3.187664  |
| Sb | -1.43135  | 1.970085  | 3.187664  |
| Sb | 0         | -3.94017  | 0.752505  |
| Sb | -2.315974 | -3.187664 | -0.752505 |
| Sb | -3.747324 | -1.217579 | 0.752505  |
| Sb | 2.315974  | -3.187664 | -0.752505 |
| Sb | 3.747324  | -1.217579 | 0.752505  |
| Sb | 3.747324  | 1.217579  | -0.752505 |
| Sb | 2.315974  | 3.187664  | 0.752505  |
| Sb | 0         | 3.94017   | -0.752505 |
| Sb | -2.315974 | 3.187664  | 0.752505  |
| Sb | -3.747324 | 1.217579  | -0.752505 |
| Sb | 1.43135   | -1.970085 | -3.187664 |
| Sb | 2.315974  | 0.752505  | -3.187664 |
| Sb | 0         | 2.435159  | -3.187664 |
| Sb | -2.315974 | 0.752505  | -3.187664 |
| Sb | -1.43135  | -1.970085 | -3.187664 |

Bi<sub>20</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| Bi | -2.414939 | -0.784661 | 3.323879  |
| Bi | 0         | -2.539217 | 3.323879  |
| Bi | 2.414939  | -0.784661 | 3.323879  |
| Bi | 1.492515  | 2.05427   | 3.323879  |
| Bi | -1.492515 | 2.05427   | 3.323879  |
| Bi | 0         | -4.10854  | 0.784661  |
| Bi | -2.414939 | -3.323879 | -0.784661 |
| Bi | -3.907454 | -1.269609 | 0.784661  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Bi | 2.414939  | -3.323879 | -0.784661 |
| Bi | 3.907454  | -1.269609 | 0.784661  |
| Bi | 3.907454  | 1.269609  | -0.784661 |
| Bi | 2.414939  | 3.323879  | 0.784661  |
| Bi | 0         | 4.10854   | -0.784661 |
| Bi | -2.414939 | 3.323879  | 0.784661  |
| Bi | -3.907454 | 1.269609  | -0.784661 |
| Bi | 1.492515  | -2.05427  | -3.323879 |
| Bi | 2.414939  | 0.784661  | -3.323879 |
| Bi | 0         | 2.539217  | -3.323879 |
| Bi | -2.414939 | 0.784661  | -3.323879 |
| Bi | -1.492515 | -2.05427  | -3.323879 |

Bi<sub>20</sub>  $\subset$  He

|    |           |           |           |
|----|-----------|-----------|-----------|
| He | 0         | 0         | 0         |
| Bi | -2.415105 | -0.784715 | 3.324106  |
| Bi | 0         | -2.539391 | 3.324106  |
| Bi | 2.415105  | -0.784715 | 3.324106  |
| Bi | 1.492617  | 2.054411  | 3.324106  |
| Bi | -1.492617 | 2.054411  | 3.324106  |
| Bi | 0         | -4.108821 | 0.784715  |
| Bi | -2.415105 | -3.324106 | -0.784715 |
| Bi | -3.907721 | -1.269696 | 0.784715  |
| Bi | 2.415105  | -3.324106 | -0.784715 |
| Bi | 3.907721  | -1.269696 | 0.784715  |
| Bi | 3.907721  | 1.269696  | -0.784715 |
| Bi | 2.415105  | 3.324106  | 0.784715  |
| Bi | 0         | 4.108821  | -0.784715 |
| Bi | -2.415105 | 3.324106  | 0.784715  |
| Bi | -3.907721 | 1.269696  | -0.784715 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Bi | 1.492617  | -2.054411 | -3.324106 |
| Bi | 2.415105  | 0.784715  | -3.324106 |
| Bi | 0         | 2.539391  | -3.324106 |
| Bi | -2.415105 | 0.784715  | -3.324106 |
| Bi | -1.492617 | -2.054411 | -3.324106 |

Bi<sub>20</sub> ⊂ Ne

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ne | 0         | 0         | 0         |
| Bi | -2.414444 | -0.7845   | 3.323197  |
| Bi | 0         | -2.538697 | 3.323197  |
| Bi | 2.414444  | -0.7845   | 3.323197  |
| Bi | 1.492208  | 2.053849  | 3.323197  |
| Bi | -1.492208 | 2.053849  | 3.323197  |
| Bi | 0         | -4.107697 | 0.7845    |
| Bi | -2.414444 | -3.323197 | -0.7845   |
| Bi | -3.906652 | -1.269348 | 0.7845    |
| Bi | 2.414444  | -3.323197 | -0.7845   |
| Bi | 3.906652  | -1.269348 | 0.7845    |
| Bi | 3.906652  | 1.269348  | -0.7845   |
| Bi | 2.414444  | 3.323197  | 0.7845    |
| Bi | 0         | 4.107697  | -0.7845   |
| Bi | -2.414444 | 3.323197  | 0.7845    |
| Bi | -3.906652 | 1.269348  | -0.7845   |
| Bi | 1.492208  | -2.053849 | -3.323197 |
| Bi | 2.414444  | 0.7845    | -3.323197 |
| Bi | 0         | 2.538697  | -3.323197 |
| Bi | -2.414444 | 0.7845    | -3.323197 |
| Bi | -1.492208 | -2.053849 | -3.323197 |

Bi<sub>20</sub> ⊂ Ar

|    |           |           |           |
|----|-----------|-----------|-----------|
| Ar | 0         | 0         | 0         |
| Bi | -2.415875 | -0.784965 | 3.325167  |
| Bi | 0         | -2.540201 | 3.325167  |
| Bi | 2.415875  | -0.784965 | 3.325167  |
| Bi | 1.493093  | 2.055066  | 3.325167  |
| Bi | -1.493093 | 2.055066  | 3.325167  |
| Bi | 0         | -4.110132 | 0.784965  |
| Bi | -2.415875 | -3.325167 | -0.784965 |
| Bi | -3.908968 | -1.270101 | 0.784965  |
| Bi | 2.415875  | -3.325167 | -0.784965 |
| Bi | 3.908968  | -1.270101 | 0.784965  |
| Bi | 3.908968  | 1.270101  | -0.784965 |
| Bi | 2.415875  | 3.325167  | 0.784965  |
| Bi | 0         | 4.110132  | -0.784965 |
| Bi | -2.415875 | 3.325167  | 0.784965  |
| Bi | -3.908968 | 1.270101  | -0.784965 |
| Bi | 1.493093  | -2.055066 | -3.325167 |
| Bi | 2.415875  | 0.784965  | -3.325167 |
| Bi | 0         | 2.540201  | -3.325167 |
| Bi | -2.415875 | 0.784965  | -3.325167 |
| Bi | -1.493093 | -2.055066 | -3.325167 |

$\text{Bi}_{20} \subset \text{Kr}$

|    |           |           |          |
|----|-----------|-----------|----------|
| Kr | 0         | 0         | 0        |
| Bi | -2.420488 | -0.786464 | 3.331516 |
| Bi | 0         | -2.545052 | 3.331516 |
| Bi | 2.420488  | -0.786464 | 3.331516 |
| Bi | 1.495944  | 2.05899   | 3.331516 |
| Bi | -1.495944 | 2.05899   | 3.331516 |
| Bi | 0         | -4.11798  | 0.786464 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Bi | -2.420488 | -3.331516 | -0.786464 |
| Bi | -3.916432 | -1.272526 | 0.786464  |
| Bi | 2.420488  | -3.331516 | -0.786464 |
| Bi | 3.916432  | -1.272526 | 0.786464  |
| Bi | 3.916432  | 1.272526  | -0.786464 |
| Bi | 2.420488  | 3.331516  | 0.786464  |
| Bi | 0         | 4.11798   | -0.786464 |
| Bi | -2.420488 | 3.331516  | 0.786464  |
| Bi | -3.916432 | 1.272526  | -0.786464 |
| Bi | 1.495944  | -2.05899  | -3.331516 |
| Bi | 2.420488  | 0.786464  | -3.331516 |
| Bi | 0         | 2.545052  | -3.331516 |
| Bi | -2.420488 | 0.786464  | -3.331516 |
| Bi | -1.495944 | -2.05899  | -3.331516 |

Bi<sub>20</sub> ⊂ Xe

|    |           |           |           |
|----|-----------|-----------|-----------|
| Xe | 0         | 0         | 0         |
| Bi | -2.427353 | -0.788695 | 3.340965  |
| Bi | 0         | -2.55227  | 3.340965  |
| Bi | 2.427353  | -0.788695 | 3.340965  |
| Bi | 1.500187  | 2.06483   | 3.340965  |
| Bi | -1.500187 | 2.06483   | 3.340965  |
| Bi | 0         | -4.12966  | 0.788695  |
| Bi | -2.427353 | -3.340965 | -0.788695 |
| Bi | -3.92754  | -1.276135 | 0.788695  |
| Bi | 2.427353  | -3.340965 | -0.788695 |
| Bi | 3.92754   | -1.276135 | 0.788695  |
| Bi | 3.92754   | 1.276135  | -0.788695 |
| Bi | 2.427353  | 3.340965  | 0.788695  |
| Bi | 0         | 4.12966   | -0.788695 |

|    |           |          |           |
|----|-----------|----------|-----------|
| Bi | -2.427353 | 3.340965 | 0.788695  |
| Bi | -3.92754  | 1.276135 | -0.788695 |
| Bi | 1.500187  | -2.06483 | -3.340965 |
| Bi | 2.427353  | 0.788695 | -3.340965 |
| Bi | 0         | 2.55227  | -3.340965 |
| Bi | -2.427353 | 0.788695 | -3.340965 |
| Bi | -1.500187 | -2.06483 | -3.340965 |

$\text{Bi}_{20} \subset \text{Rn}$

|    |           |           |           |
|----|-----------|-----------|-----------|
| Rn | 0         | 0         | 0         |
| Bi | -2.432004 | -0.790206 | 3.347367  |
| Bi | 0         | -2.557161 | 3.347367  |
| Bi | 2.432004  | -0.790206 | 3.347367  |
| Bi | 1.503061  | 2.068786  | 3.347367  |
| Bi | -1.503061 | 2.068786  | 3.347367  |
| Bi | 0         | -4.137573 | 0.790206  |
| Bi | -2.432004 | -3.347367 | -0.790206 |
| Bi | -3.935066 | -1.27858  | 0.790206  |
| Bi | 2.432004  | -3.347367 | -0.790206 |
| Bi | 3.935066  | -1.27858  | 0.790206  |
| Bi | 3.935066  | 1.27858   | -0.790206 |
| Bi | 2.432004  | 3.347367  | 0.790206  |
| Bi | 0         | 4.137573  | -0.790206 |
| Bi | -2.432004 | 3.347367  | 0.790206  |
| Bi | -3.935066 | 1.27858   | -0.790206 |
| Bi | 1.503061  | -2.068786 | -3.347367 |
| Bi | 2.432004  | 0.790206  | -3.347367 |
| Bi | 0         | 2.557161  | -3.347367 |
| Bi | -2.432004 | 0.790206  | -3.347367 |
| Bi | -1.503061 | -2.068786 | -3.347367 |

Table S2. Number of imaginary frequencies calculated at the  $\omega$ B97XD/ def2-svp/svpfit theory level for X<sub>20</sub>H<sub>20</sub> host

| Noble gas | C     | Si             | Ge    | Sn    | Pb                 |
|-----------|-------|----------------|-------|-------|--------------------|
|           | Nimag | Nimag          | Nimag | Nimag | Nimag              |
| empty     | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |
| He        | 0     | 3 <sup>§</sup> | 0     | 0     | 8 <sup>&amp;</sup> |
| Ne        | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |
| Ar        | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |
| Kr        | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |
| Xe        | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |
| Rn        | 0     | 0              | 0     | 0     | 8 <sup>&amp;</sup> |

<sup>§</sup>Noble gas is moving inside the cage's cavity for comparability noted altered to lower symmetry

<sup>&</sup>The Pb<sub>20</sub>H<sub>20</sub> skeleton undergoes small vibrations, elongating them and recalculating without symmetry leading to slightly distorted pentagonal dodecahedral structures. For comparability the reported systems with higher symmetry were selected.

Table S3. Number of imaginary frequencies calculated at the  $\omega$ B97XD/ def2-svp/svpfit theory level for X<sub>20</sub> host

| Noble gas | N                   | P     | As             | Sb    | Bi    |
|-----------|---------------------|-------|----------------|-------|-------|
|           | Nimag               | Nimag | Nimag          | Nimag | Nimag |
| empty     | 0                   | 0     | 0              | 0     | 0     |
| He        | 0                   | 0     | 3 <sup>§</sup> | 0     | 0     |
| Ne        | 0                   | 0     | 0              | 0     | 0     |
| Ar        | 0                   | 0     | 0              | 0     | 0     |
| Kr        | 13 <sup>&amp;</sup> | 0     | 0              | 0     | 0     |
| Xe        | 17 <sup>&amp;</sup> | 0     | 0              | 0     | 0     |
| Rn        | 23 <sup>&amp;</sup> | 0     | 0              | 0     | 0     |

<sup>§</sup> Noble gas is moving inside the cage's cavity for comparability noted altered to lower symmetry

<sup>&</sup> Noble gases of a relatively bigger radii are too small for the selected hosts cavity

Table S4. Number of imaginary frequencies calculated on different theory levels for the Pb<sub>20</sub>H<sub>20</sub> and Bi<sub>20</sub> hosts.

| Noble gas | Pb <sub>20</sub> H <sub>20</sub> <sup>a</sup> | Bi <sub>20</sub> <sup>a</sup> | Pb <sub>20</sub> H <sub>20</sub> <sup>b</sup> | Bi <sub>20</sub> <sup>b</sup> |
|-----------|---|-------------------------------|---|-------------------------------|
| empty     | 8   | 0                             | 8   | 0                             |
| He        | 8   | 0                             | 8   | 0                             |
| Ne        | 8   | 0                             | 8   | 0                             |

|    |   |   |   |   |
|----|---|---|---|---|
| Ar | 8 | 0 | 8 | 0 |
| Kr | 8 | 0 | 8 | 0 |
| Xe | 8 | 0 | 8 | 0 |
| Rn | 8 | 0 | 8 | 0 |

<sup>a</sup>APFD/def2-svp/svpfit

<sup>b</sup>B3LYP- GD3BJ /def2-svp/svpfit

Table S5. Gaussian keywords input templates for the performed calculations.

#P Rwb97XD/def2svp/svpfit opt freq=noraman

#P APFD/def2svp/svpfit opt freq=noraman

#P RB3LYP/ def2svp/svpfit EmpiricalDispersion=GD3BJ opt freq=noraman

#P Rwb97XD/def2svp/def2-tzvp

#P test Rwb97XD/def2tzvp Counterpoise=2

0,1 0,1 0,1

Ng(Fragment=1)

Cage(Fragment=2)

....

#P Rwb97XD/def2tzvp POP=chelp

#P Rwb97XD/def2svp/def2-tzvp

#P RAPFD/def2tzvp

#P RB3LYP/def2tzvp EmpiricalDispersion=GD3BJ

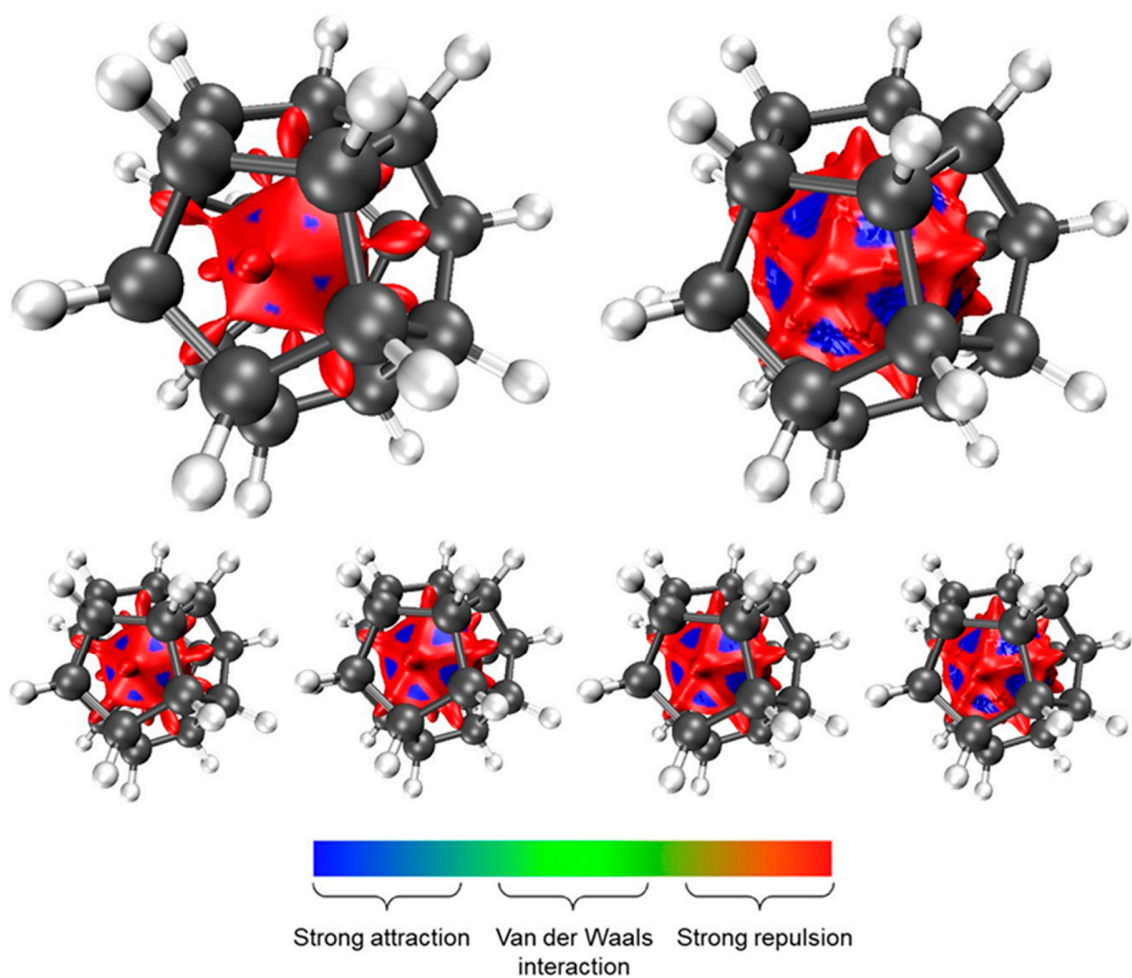


Figure S1. Structure of  $C_{20}H_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.18). Top row: He and Rn. Bottom row: Ne, Ar, Kr and Xe.

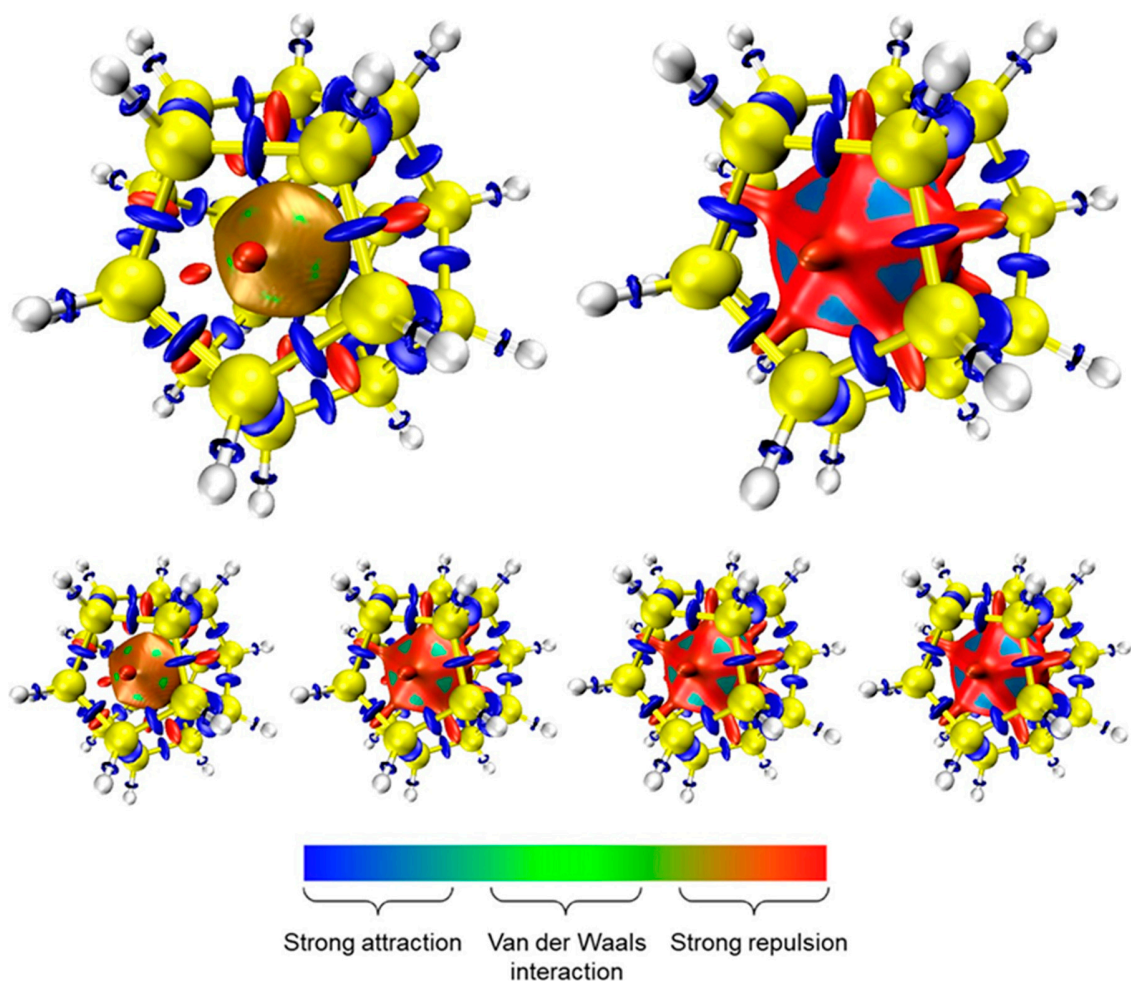


Figure S2. Structure of  $\text{Si}_{20}\text{H}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.22). Top row: He and Rn. Bottom row: Ne, Ar, Kr and Xe.

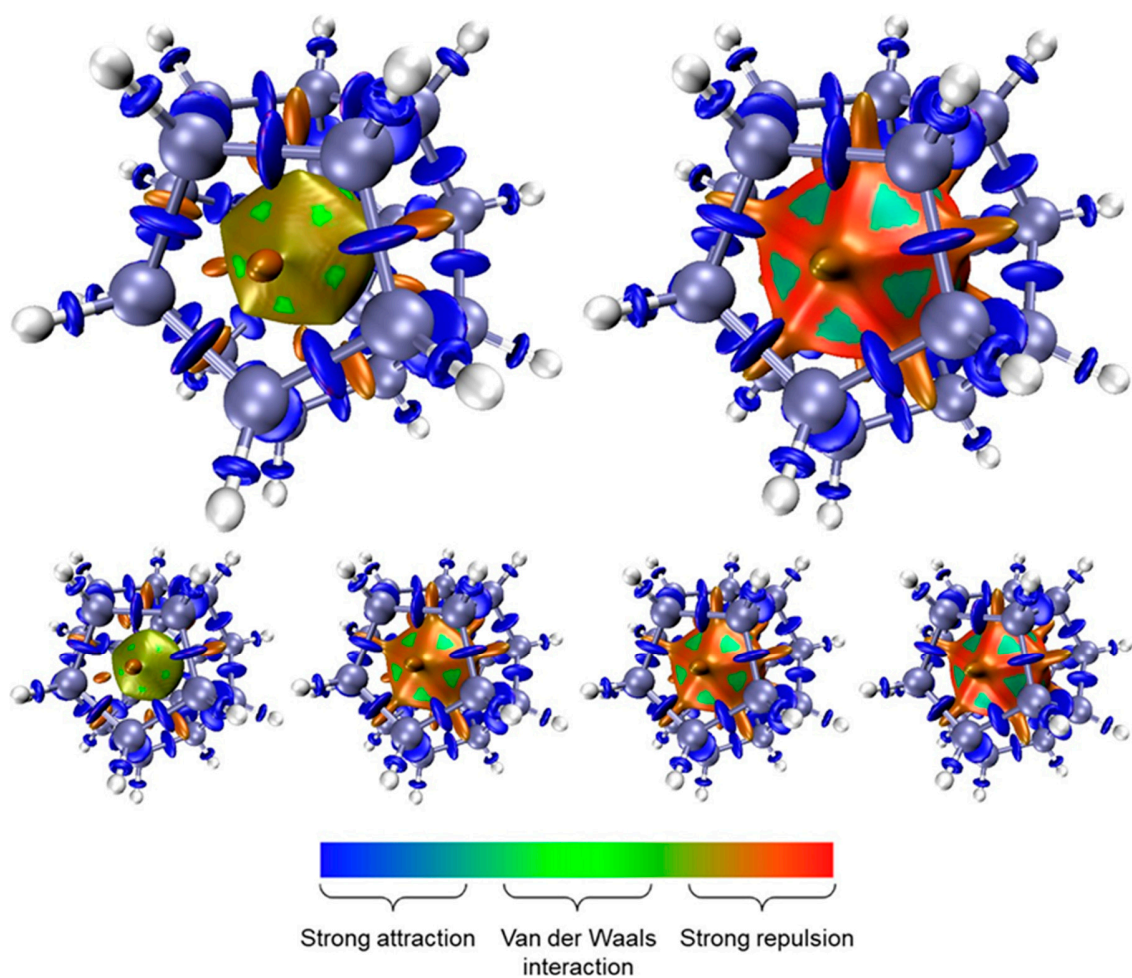


Figure S3. Structure of  $\text{Ge}_{20}\text{H}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.3). Top row: Ne and Rn. Bottom row: He, Ar, Kr and Xe.

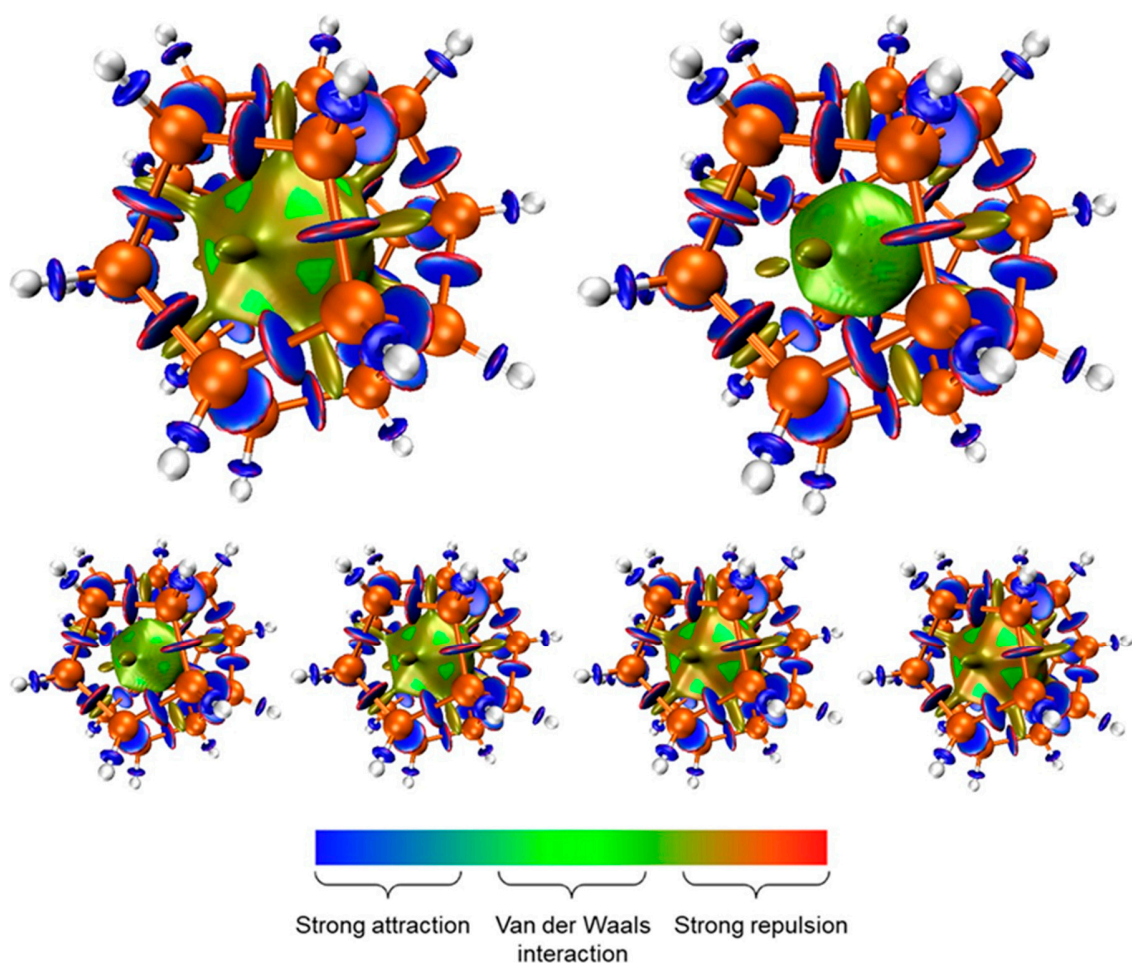


Figure S4. Structure of  $\text{Sn}_{20}\text{H}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.35). Top row: Kr and He. Bottom row: Ne, Ar, Xe and Rn.

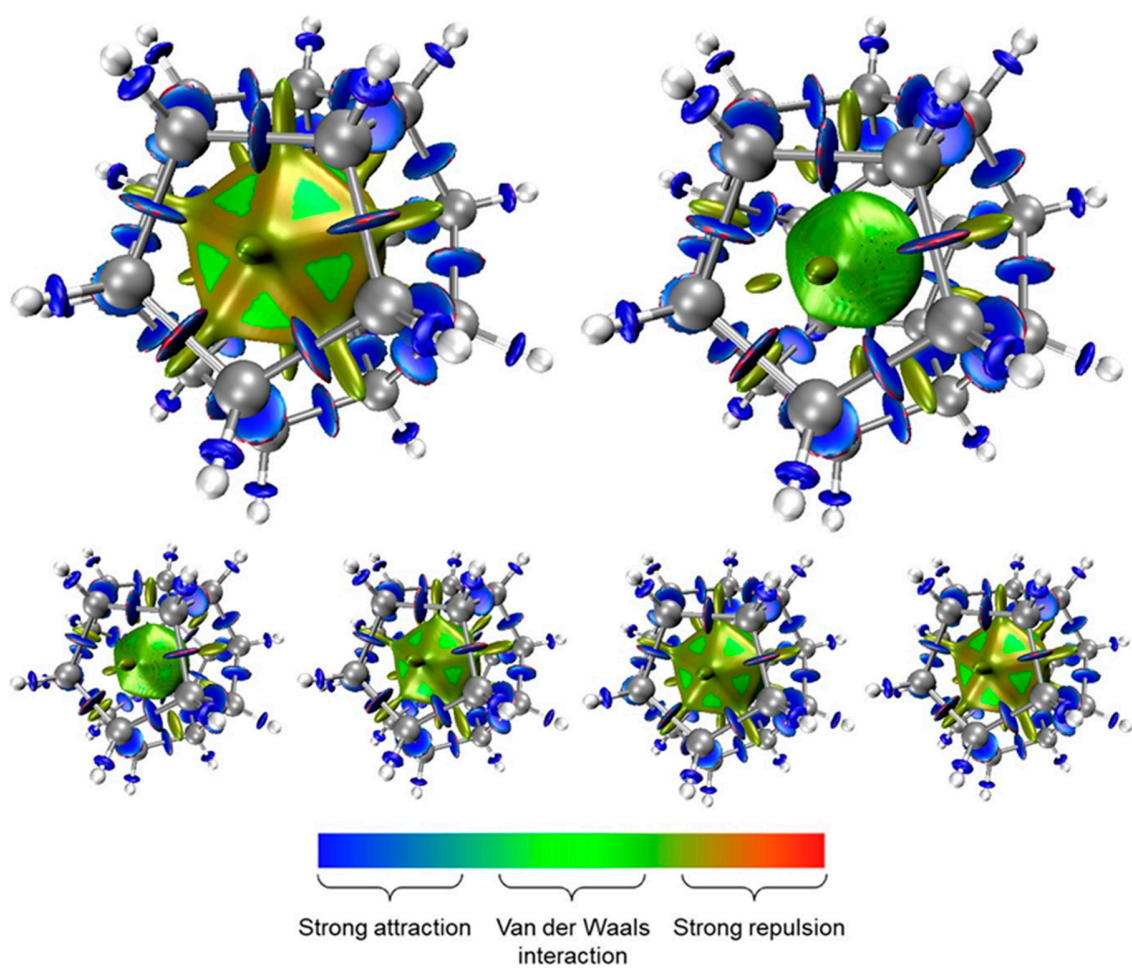


Figure S5. Structure of  $\text{Pb}_{20}\text{H}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.35). Top row: Rn and He. Bottom row: Ne, Ar, Kr and Xe.

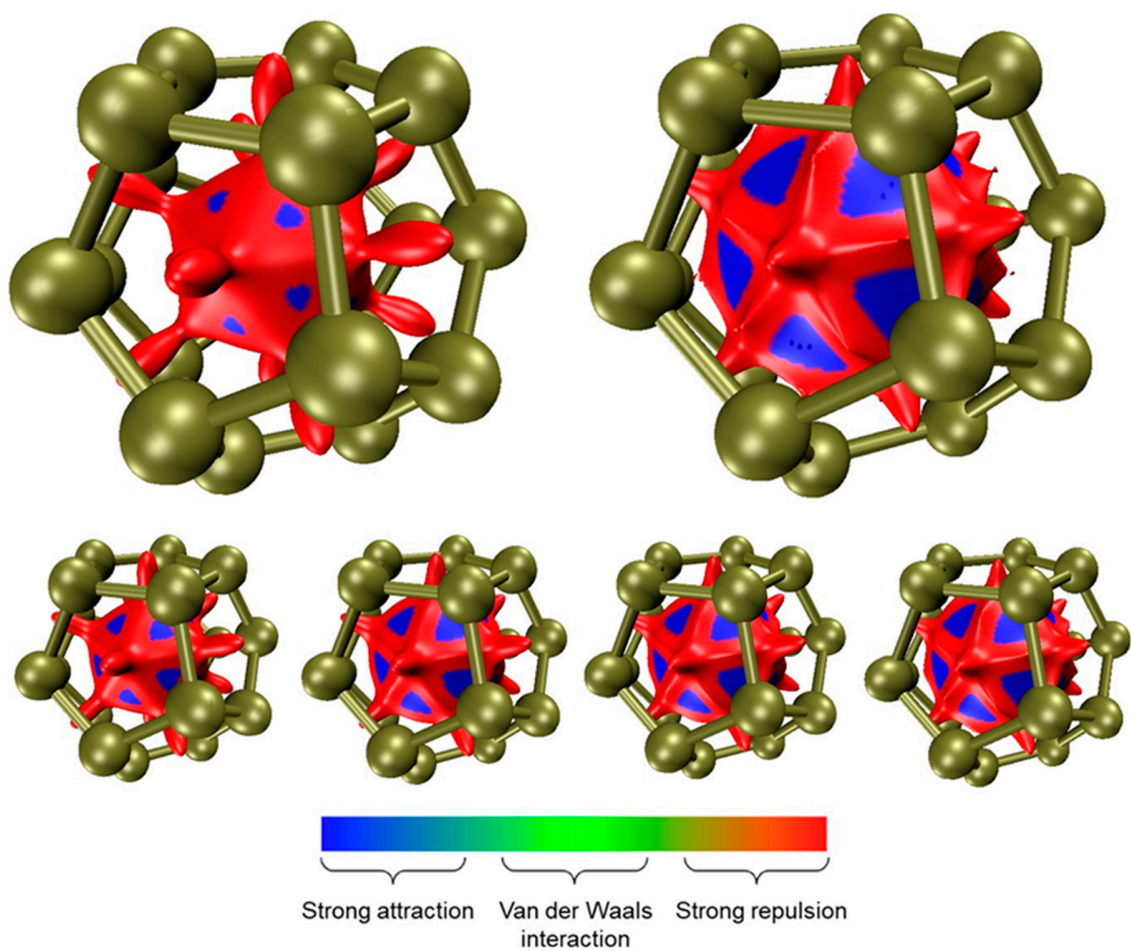


Figure S6. Structure of  $N_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.25). Top row: He and Rn. Bottom row: Ne, Ar, Kr and Xe.

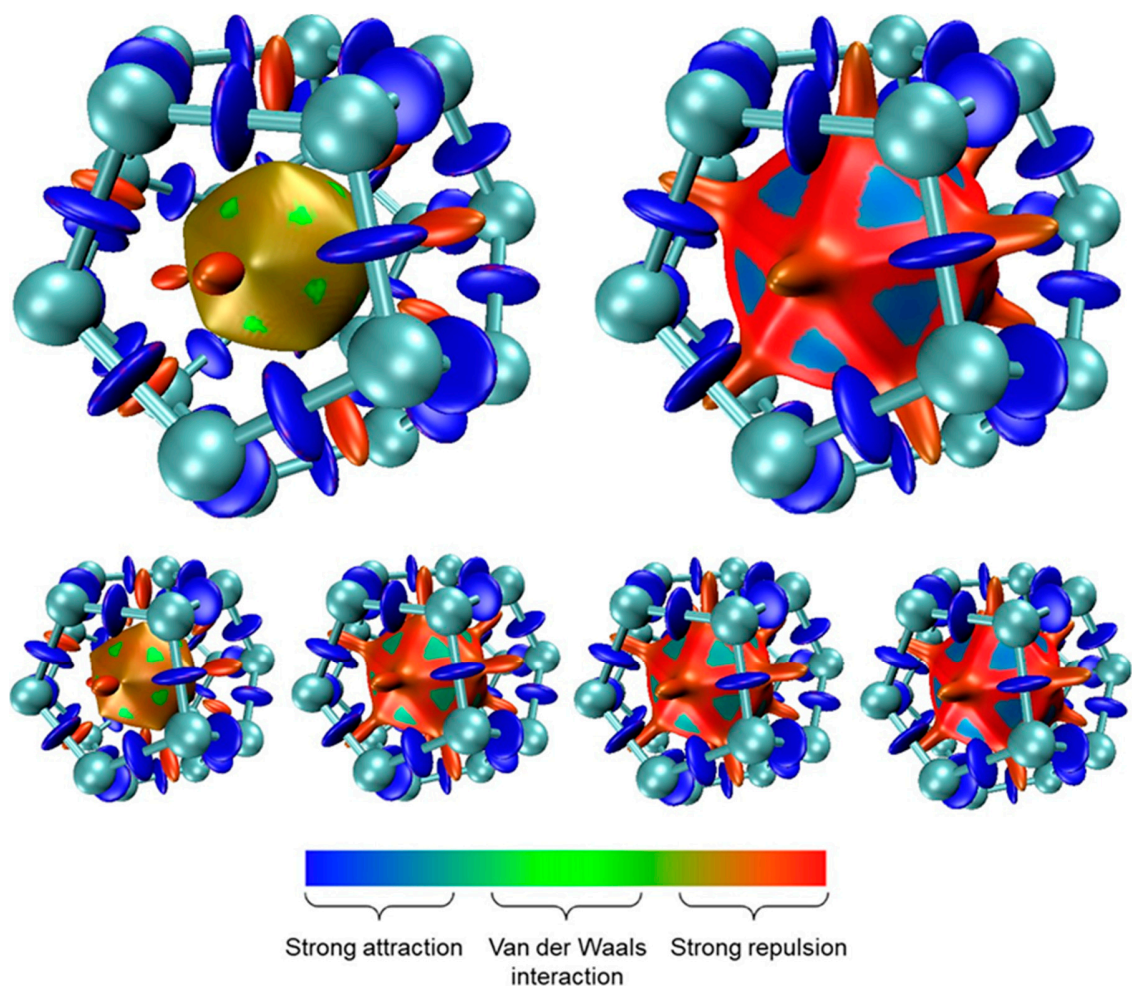


Figure S7. Structure of  $P_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.3). Top row: He and Rn. Bottom row: Ne, Ar, Kr and Xe.

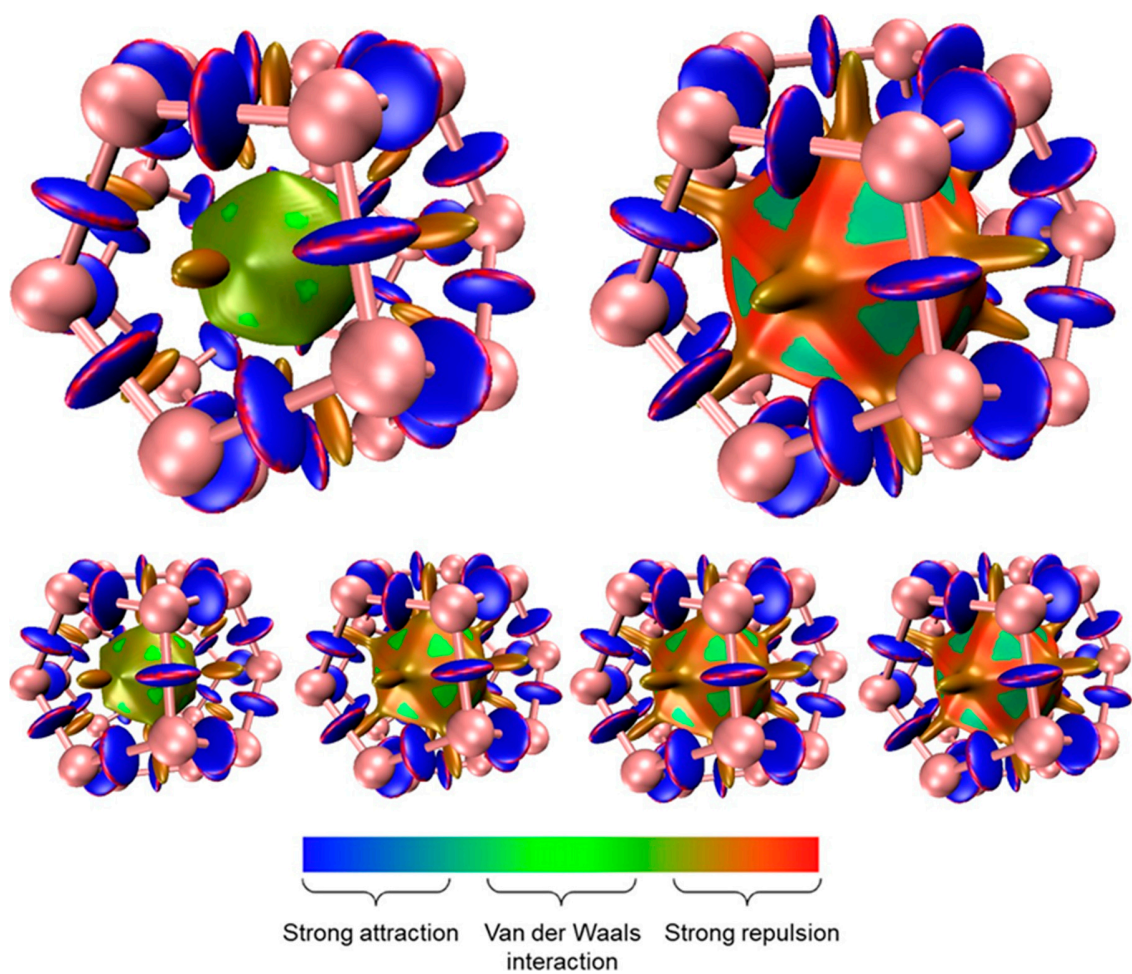


Figure S8. Structure of  $\text{As}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.35). Top row: He and Rn. Bottom row: Ne, Ar, Kr and Xe.

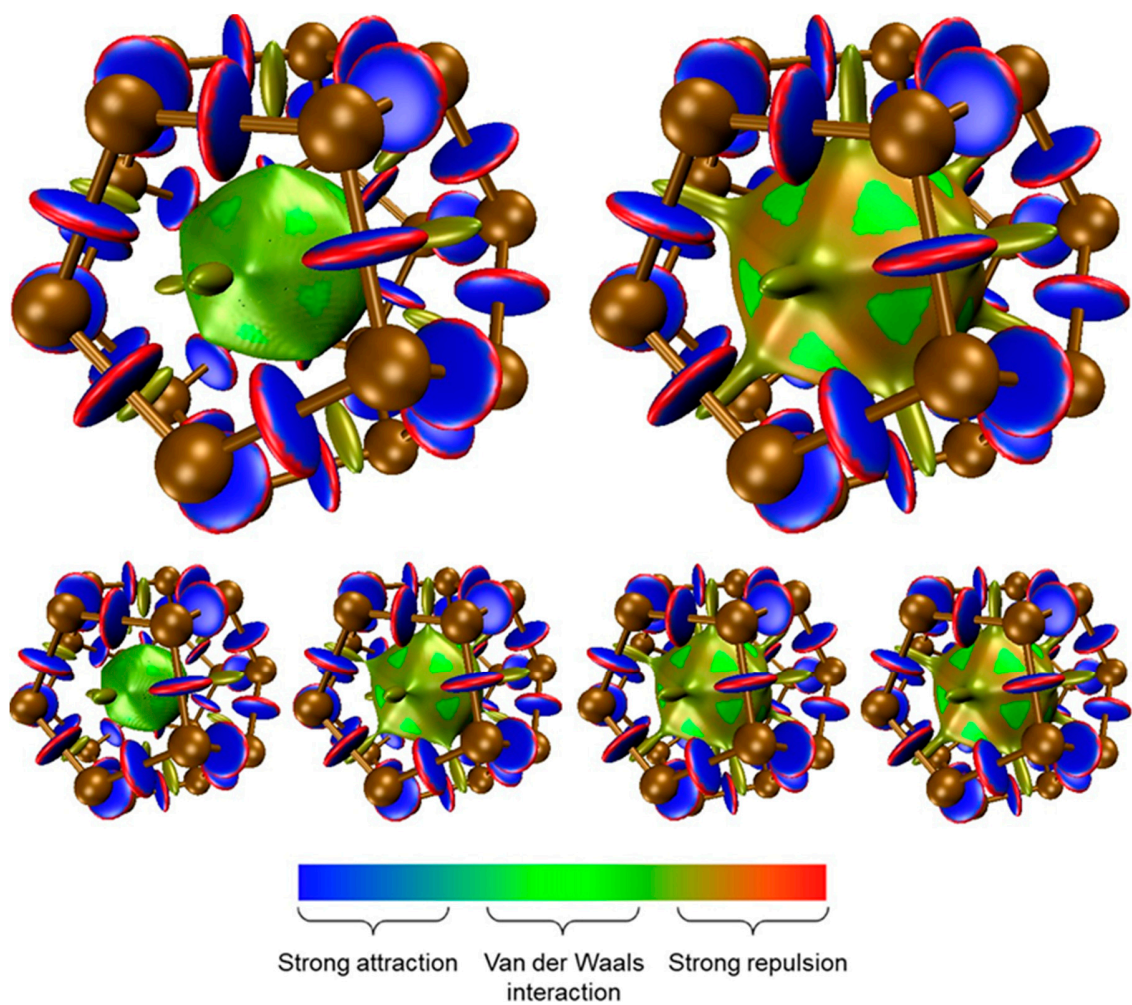


Figure S9. Structure of  $\text{Sb}_{20}$  with displayed non-covalent interactions according to the color bar (isoval = 0.37). Top row: Ne and Rn. Bottom row: He, Ar, Kr and Xe.