

## SUPPORTING INFORMATION

### Silver cluster doped graphene (GY) with outstanding non-linear optical properties

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**Optimized cartesian coordinates for the geometry of doped complexes (GY@Ag<sub>center</sub>**

**- GY@3Ag<sub>center</sub>) and pure GY as well as (2GY@Ag<sub>center</sub> - 2GY@3Ag<sub>center</sub>)**

### Complexes of Model 1

**GY@Ag<sub>center</sub>**

| Center Number | Atomic Number | Atomic Type | X         | Y         | Z        |
|---------------|---------------|-------------|-----------|-----------|----------|
| 1             | 6             | 0           | -4.608811 | -1.554959 | 0        |
| 2             | 6             | 0           | -3.21365  | -1.55496  | 0        |
| 3             | 6             | 0           | -2.51611  | -0.34721  | 0        |
| 4             | 6             | 0           | -3.21377  | 0.861301  | -0.0012  |
| 5             | 6             | 0           | -4.60859  | 0.861223  | -0.00168 |
| 6             | 6             | 0           | -5.30619  | -0.34698  | -0.00068 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 7  | 1  | 0 | -5.15857 | -2.50728 | 0.00045  |
| 8  | 1  | 0 | -2.66414 | -2.50747 | 0.001315 |
| 9  | 1  | 0 | -5.15871 | 1.813504 | -0.00263 |
| 10 | 1  | 0 | -6.4058  | -0.3468  | -0.00086 |
| 11 | 6  | 0 | 3.178829 | -1.53611 | -0.02352 |
| 12 | 6  | 0 | 4.573989 | -1.53611 | -0.02352 |
| 13 | 6  | 0 | 5.271527 | -0.32836 | -0.02352 |
| 14 | 6  | 0 | 4.573873 | 0.880151 | -0.02471 |
| 15 | 6  | 0 | 3.179048 | 0.880073 | -0.02519 |
| 16 | 6  | 0 | 2.481447 | -0.32813 | -0.0242  |
| 17 | 1  | 0 | 2.62907  | -2.48843 | -0.02307 |
| 18 | 1  | 0 | 5.123497 | -2.48862 | -0.0222  |
| 19 | 1  | 0 | 6.371207 | -0.32828 | -0.02288 |
| 20 | 1  | 0 | 5.124073 | 1.832294 | -0.02477 |
| 21 | 6  | 0 | -0.67967 | 4.915796 | 0.044884 |
| 22 | 6  | 0 | 0.715486 | 4.915796 | 0.044884 |
| 23 | 6  | 0 | 1.413024 | 6.123547 | 0.044884 |
| 24 | 6  | 0 | 0.71537  | 7.332056 | 0.043685 |
| 25 | 6  | 0 | -0.67946 | 7.331978 | 0.043206 |
| 26 | 6  | 0 | -1.37706 | 6.123772 | 0.044202 |
| 27 | 1  | 0 | 2.512704 | 6.123627 | 0.045518 |
| 28 | 1  | 0 | 1.26557  | 8.284199 | 0.043626 |
| 29 | 1  | 0 | -1.22958 | 8.284259 | 0.042253 |
| 30 | 1  | 0 | -2.47666 | 6.123955 | 0.044022 |
| 31 | 6  | 0 | -2.44326 | 2.194689 | -0.00128 |
| 32 | 6  | 0 | -0.97611 | -0.3471  | 0.000888 |
| 33 | 6  | 0 | 0.941447 | -0.32788 | -0.02445 |
| 34 | 6  | 0 | 2.40871  | 2.213556 | -0.02653 |
| 35 | 6  | 0 | -1.44961 | 3.58208  | 0.045515 |
| 36 | 6  | 0 | 1.485038 | 3.58186  | 0.046726 |
| 37 | 47 | 0 | 0.093488 | 1.96424  | -1.62517 |

**GY@Ag<sub>side</sub>**

| Center Number | Atomic Number | Atomic Type | X         | Y         | Z        |
|---------------|---------------|-------------|-----------|-----------|----------|
| 1             | 6             | 0           | -4.608811 | -1.554959 | 0        |
| 2             | 6             | 0           | -3.21365  | -1.55496  | 0        |
| 3             | 6             | 0           | -2.51611  | -0.34721  | 0        |
| 4             | 6             | 0           | -3.21377  | 0.861301  | -0.0012  |
| 5             | 6             | 0           | -4.60859  | 0.861223  | -0.00168 |
| 6             | 6             | 0           | -5.30619  | -0.34698  | -0.00068 |
| 7             | 1             | 0           | -5.15857  | -2.50728  | 0.00045  |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 8  | 1  | 0 | -2.66414 | -2.50747 | 0.001315 |
| 9  | 1  | 0 | -5.15871 | 1.813504 | -0.00263 |
| 10 | 1  | 0 | -6.4058  | -0.3468  | -0.00086 |
| 11 | 6  | 0 | 3.178829 | -1.53611 | -0.02352 |
| 12 | 6  | 0 | 4.573989 | -1.53611 | -0.02352 |
| 13 | 6  | 0 | 5.271527 | -0.32836 | -0.02352 |
| 14 | 6  | 0 | 4.573873 | 0.880151 | -0.02471 |
| 15 | 6  | 0 | 3.179048 | 0.880073 | -0.02519 |
| 16 | 6  | 0 | 2.481447 | -0.32813 | -0.0242  |
| 17 | 1  | 0 | 2.62907  | -2.48843 | -0.02307 |
| 18 | 1  | 0 | 5.123497 | -2.48862 | -0.0222  |
| 19 | 1  | 0 | 6.371207 | -0.32828 | -0.02288 |
| 20 | 1  | 0 | 5.124073 | 1.832294 | -0.02477 |
| 21 | 6  | 0 | -0.67967 | 4.915796 | 0.044884 |
| 22 | 6  | 0 | 0.715486 | 4.915796 | 0.044884 |
| 23 | 6  | 0 | 1.413024 | 6.123547 | 0.044884 |
| 24 | 6  | 0 | 0.71537  | 7.332056 | 0.043685 |
| 25 | 6  | 0 | -0.67946 | 7.331978 | 0.043206 |
| 26 | 6  | 0 | -1.37706 | 6.123772 | 0.044202 |
| 27 | 1  | 0 | 2.512704 | 6.123627 | 0.045518 |
| 28 | 1  | 0 | 1.26557  | 8.284199 | 0.043626 |
| 29 | 1  | 0 | -1.22958 | 8.284259 | 0.042253 |
| 30 | 1  | 0 | -2.47666 | 6.123955 | 0.044022 |
| 31 | 6  | 0 | -2.44326 | 2.194689 | -0.00128 |
| 32 | 6  | 0 | -0.97611 | -0.3471  | 0.000888 |
| 33 | 6  | 0 | 0.941447 | -0.32788 | -0.02445 |
| 34 | 6  | 0 | 2.40871  | 2.213556 | -0.02653 |
| 35 | 6  | 0 | -1.44961 | 3.58208  | 0.045515 |
| 36 | 6  | 0 | 1.485038 | 3.58186  | 0.046726 |
| 37 | 47 | 0 | 3.955306 | -0.22946 | -1.31013 |

**GY@2Ag<sub>perpendicular</sub>**

| Center Number | Atomic Number | Atomic Type | X         | Y         | Z         |
|---------------|---------------|-------------|-----------|-----------|-----------|
| 1             | 6             | 0           | -4.439564 | -1.702097 | -0.100663 |
| 2             | 6             | 0           | -3.0444   | -1.7021   | -0.10066  |
| 3             | 6             | 0           | -2.34687  | -0.49435  | -0.10066  |
| 4             | 6             | 0           | -3.04452  | 0.714163  | -0.10186  |
| 5             | 6             | 0           | -4.43935  | 0.714085  | -0.10234  |
| 6             | 6             | 0           | -5.13695  | -0.49412  | -0.10135  |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 7  | 1  | 0 | -4.98932 | -2.65441 | -0.10021 |
| 8  | 1  | 0 | -2.4949  | -2.65461 | -0.09935 |
| 9  | 1  | 0 | -4.98947 | 1.666366 | -0.10329 |
| 10 | 1  | 0 | -6.23655 | -0.49394 | -0.10153 |
| 11 | 6  | 0 | 3.348076 | -1.68325 | -0.12418 |
| 12 | 6  | 0 | 4.743236 | -1.68325 | -0.12418 |
| 13 | 6  | 0 | 5.440774 | -0.4755  | -0.12418 |
| 14 | 6  | 0 | 4.74312  | 0.733013 | -0.12538 |
| 15 | 6  | 0 | 3.348295 | 0.732935 | -0.12586 |
| 16 | 6  | 0 | 2.650694 | -0.47527 | -0.12486 |
| 17 | 1  | 0 | 2.798317 | -2.63556 | -0.12373 |
| 18 | 1  | 0 | 5.292744 | -2.63576 | -0.12286 |
| 19 | 1  | 0 | 6.540454 | -0.47542 | -0.12354 |
| 20 | 1  | 0 | 5.29332  | 1.685156 | -0.12544 |
| 21 | 6  | 0 | -0.51043 | 4.768658 | -0.05578 |
| 22 | 6  | 0 | 0.884733 | 4.768658 | -0.05578 |
| 23 | 6  | 0 | 1.582271 | 5.976409 | -0.05578 |
| 24 | 6  | 0 | 0.884617 | 7.184918 | -0.05698 |
| 25 | 6  | 0 | -0.51021 | 7.18484  | -0.05746 |
| 26 | 6  | 0 | -1.20781 | 5.976634 | -0.05646 |
| 27 | 1  | 0 | 2.681951 | 5.976489 | -0.05515 |
| 28 | 1  | 0 | 1.434817 | 8.137061 | -0.05704 |
| 29 | 1  | 0 | -1.06033 | 8.137121 | -0.05841 |
| 30 | 1  | 0 | -2.30741 | 5.976817 | -0.05664 |
| 31 | 6  | 0 | -2.27402 | 2.047551 | -0.10194 |
| 32 | 6  | 0 | -0.80687 | -0.49423 | -0.09978 |
| 33 | 6  | 0 | 1.110694 | -0.47501 | -0.12511 |
| 34 | 6  | 0 | 2.577957 | 2.066419 | -0.12719 |
| 35 | 6  | 0 | -1.28036 | 3.434942 | -0.05515 |
| 36 | 6  | 0 | 1.654285 | 3.434722 | -0.05394 |
| 37 | 47 | 0 | 0.243013 | 1.549342 | -1.3091  |
| 38 | 47 | 0 | 0.209061 | 1.514804 | 1.370467 |

**GY@2A<sub>g</sub>above**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | -4.43956 | -1.7021  | -0.10066 |
| 2             | 6             | 0           | -3.0444  | -1.7021  | -0.10066 |
| 3             | 6             | 0           | -2.34687 | -0.49435 | -0.10066 |
| 4             | 6             | 0           | -3.04452 | 0.714163 | -0.10186 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 5  | 6  | 0 | -4.43935 | 0.714085 | -0.10234 |
| 6  | 6  | 0 | -5.13695 | -0.49412 | -0.10135 |
| 7  | 1  | 0 | -4.98932 | -2.65441 | -0.10021 |
| 8  | 1  | 0 | -2.4949  | -2.65461 | -0.09935 |
| 9  | 1  | 0 | -4.98947 | 1.666366 | -0.10329 |
| 10 | 1  | 0 | -6.23655 | -0.49394 | -0.10153 |
| 11 | 6  | 0 | 3.348076 | -1.68325 | -0.12418 |
| 12 | 6  | 0 | 4.743236 | -1.68325 | -0.12418 |
| 13 | 6  | 0 | 5.440774 | -0.4755  | -0.12418 |
| 14 | 6  | 0 | 4.74312  | 0.733013 | -0.12538 |
| 15 | 6  | 0 | 3.348295 | 0.732935 | -0.12586 |
| 16 | 6  | 0 | 2.650694 | -0.47527 | -0.12486 |
| 17 | 1  | 0 | 2.798317 | -2.63556 | -0.12373 |
| 18 | 1  | 0 | 5.292744 | -2.63576 | -0.12286 |
| 19 | 1  | 0 | 6.540454 | -0.47542 | -0.12354 |
| 20 | 1  | 0 | 5.29332  | 1.685156 | -0.12544 |
| 21 | 6  | 0 | -0.51043 | 4.768658 | -0.05578 |
| 22 | 6  | 0 | 0.884733 | 4.768658 | -0.05578 |
| 23 | 6  | 0 | 1.582271 | 5.976409 | -0.05578 |
| 24 | 6  | 0 | 0.884617 | 7.184918 | -0.05698 |
| 25 | 6  | 0 | -0.51021 | 7.18484  | -0.05746 |
| 26 | 6  | 0 | -1.20781 | 5.976634 | -0.05646 |
| 27 | 1  | 0 | 2.681951 | 5.976489 | -0.05515 |
| 28 | 1  | 0 | 1.434817 | 8.137061 | -0.05704 |
| 29 | 1  | 0 | -1.06033 | 8.137121 | -0.05841 |
| 30 | 1  | 0 | -2.30741 | 5.976817 | -0.05664 |
| 31 | 6  | 0 | -2.27402 | 2.047551 | -0.10194 |
| 32 | 6  | 0 | -0.80687 | -0.49423 | -0.09978 |
| 33 | 6  | 0 | 1.110694 | -0.47501 | -0.12511 |
| 34 | 6  | 0 | 2.577957 | 2.066419 | -0.12719 |
| 35 | 6  | 0 | -1.28036 | 3.434942 | -0.05515 |
| 36 | 6  | 0 | 1.654285 | 3.434722 | -0.05394 |
| 37 | 47 | 0 | -1.11618 | 1.391669 | -1.53286 |
| 38 | 47 | 0 | 1.563822 | 1.391669 | -1.53286 |

**GY@3Ag<sub>center</sub>**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 4.518496 | -0.96962 | 3.008094 |
| 2             | 6             | 0           | 3.139929 | -1.19138 | 3.072426 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 3  | 6  | 0 | 2.242326 | -0.31298 | 2.439335 |
| 4  | 6  | 0 | 2.710904 | 1.152932 | 1.579768 |
| 5  | 6  | 0 | 4.137789 | 1.01608  | 1.668534 |
| 6  | 6  | 0 | 5.018425 | 0.136325 | 2.304322 |
| 7  | 1  | 0 | 5.20107  | -1.65613 | 3.498837 |
| 8  | 1  | 0 | 2.747108 | -2.04833 | 3.609091 |
| 9  | 1  | 0 | 4.518028 | 1.868558 | 1.116079 |
| 10 | 1  | 0 | 6.088835 | 0.306993 | 2.24854  |
| 11 | 6  | 0 | -2.31806 | -1.99763 | 3.435913 |
| 12 | 6  | 0 | -3.70009 | -2.18671 | 3.530168 |
| 13 | 6  | 0 | -4.57534 | -1.31074 | 2.870579 |
| 14 | 6  | 0 | -4.06526 | -0.24763 | 2.119418 |
| 15 | 6  | 0 | -2.69855 | -0.04828 | 1.998722 |
| 16 | 6  | 0 | -1.79112 | -0.93156 | 2.685817 |
| 17 | 1  | 0 | -1.63625 | -2.67502 | 3.938631 |
| 18 | 1  | 0 | -4.0947  | -3.01454 | 4.110654 |
| 19 | 1  | 0 | -5.64815 | -1.45983 | 2.938889 |
| 20 | 1  | 0 | -4.73602 | 0.429238 | 1.601245 |
| 21 | 6  | 0 | 0.181829 | 3.400558 | -0.11452 |
| 22 | 6  | 0 | -1.21726 | 3.1584   | -0.06431 |
| 23 | 6  | 0 | -2.09803 | 4.051622 | -0.70009 |
| 24 | 6  | 0 | -1.60829 | 5.173989 | -1.3741  |
| 25 | 6  | 0 | -0.22666 | 5.414628 | -1.42319 |
| 26 | 6  | 0 | 0.660044 | 4.532386 | -0.79888 |
| 27 | 1  | 0 | -3.16438 | 3.856136 | -0.66272 |
| 28 | 1  | 0 | -2.29707 | 5.856169 | -1.86196 |
| 29 | 1  | 0 | 0.155215 | 6.283775 | -1.94923 |
| 30 | 1  | 0 | 1.729334 | 4.70985  | -0.83856 |
| 31 | 6  | 0 | 1.855745 | 1.715219 | 1.068314 |
| 32 | 6  | 0 | 0.830258 | -0.55202 | 2.510322 |
| 33 | 6  | 0 | -0.37301 | -0.74163 | 2.58623  |
| 34 | 6  | 0 | -2.10923 | 1.066107 | 1.297604 |
| 35 | 6  | 0 | 1.094145 | 2.493969 | 0.518484 |
| 36 | 6  | 0 | -1.72611 | 2.010658 | 0.629805 |
| 37 | 47 | 0 | -0.1804  | -0.22493 | -0.42993 |
| 38 | 47 | 0 | -1.19854 | -1.78768 | -2.37567 |
| 39 | 47 | 0 | 1.711783 | -0.81051 | -2.27793 |

**GY**

| <b>Center Number</b> | <b>Atomic Number</b> | <b>Atomic Type</b> | <b>X</b> | <b>Y</b> | <b>Z</b> |
|----------------------|----------------------|--------------------|----------|----------|----------|
| 1                    | 6                    | 0                  | 6.547791 | 0.701941 | -2.52358 |
| 2                    | 6                    | 0                  | 5.587028 | 1.399936 | -1.78613 |
| 3                    | 6                    | 0                  | 4.613588 | 0.710566 | -1.03978 |
| 4                    | 6                    | 0                  | 4.613657 | -0.71021 | -1.03982 |
| 5                    | 6                    | 0                  | 5.587157 | -1.39944 | -1.78622 |
| 6                    | 6                    | 0                  | 6.547855 | -0.70131 | -2.52363 |
| 7                    | 1                    | 0                  | 7.292414 | 1.245878 | -3.09618 |
| 8                    | 1                    | 0                  | 5.580404 | 2.484723 | -1.78264 |
| 9                    | 1                    | 0                  | 5.58063  | -2.48423 | -1.7828  |
| 10                   | 1                    | 0                  | 7.292526 | -1.24514 | -3.09627 |
| 11                   | 6                    | 0                  | 1.927473 | 4.101961 | 1.350735 |
| 12                   | 6                    | 0                  | 0.972422 | 4.803728 | 2.090771 |
| 13                   | 6                    | 0                  | -0.13786 | 4.13036  | 2.622988 |
| 14                   | 6                    | 0                  | -0.28439 | 2.757619 | 2.41139  |
| 15                   | 6                    | 0                  | 0.674926 | 2.039358 | 1.673626 |
| 16                   | 6                    | 0                  | 1.796206 | 2.717394 | 1.128894 |
| 17                   | 1                    | 0                  | 2.785571 | 4.618186 | 0.933936 |
| 18                   | 1                    | 0                  | 1.087843 | 5.871285 | 2.249577 |
| 19                   | 1                    | 0                  | -0.88485 | 4.673449 | 3.192575 |
| 20                   | 1                    | 0                  | -1.14681 | 2.231478 | 2.806772 |
| 21                   | 6                    | 0                  | 1.796456 | -2.71748 | 1.128678 |
| 22                   | 6                    | 0                  | 0.675068 | -2.03961 | 1.673415 |
| 23                   | 6                    | 0                  | -0.2842  | -2.75804 | 2.411068 |
| 24                   | 6                    | 0                  | -0.1375  | -4.13079 | 2.622579 |
| 25                   | 6                    | 0                  | 0.972886 | -4.80398 | 2.090379 |
| 26                   | 6                    | 0                  | 1.927885 | -4.10204 | 1.350432 |
| 27                   | 1                    | 0                  | -1.14671 | -2.23205 | 2.806444 |
| 28                   | 1                    | 0                  | -0.88446 | -4.674   | 3.192085 |
| 29                   | 1                    | 0                  | 1.088443 | -5.87153 | 2.249126 |
| 30                   | 1                    | 0                  | 2.786068 | -4.61813 | 0.933641 |
| 31                   | 6                    | 0                  | 3.632236 | -1.43256 | -0.28616 |
| 32                   | 6                    | 0                  | 3.632091 | 1.432769 | -0.28607 |
| 33                   | 6                    | 0                  | 2.786751 | 2.021269 | 0.364186 |
| 34                   | 6                    | 0                  | 0.502223 | 0.619657 | 1.481433 |
| 35                   | 6                    | 0                  | 2.786935 | -2.02118 | 0.364045 |
| 36                   | 6                    | 0                  | 0.502235 | -0.61991 | 1.48135  |

## Complexes of Model 2

2GY@Ag<sub>center</sub>

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.709412 | -1.98299 | 4.863836 |
| 2             | 6             | 0           | 2.398041 | -1.4992  | 4.868987 |
| 3             | 6             | 0           | 1.984953 | -0.52682 | 3.939172 |
| 4             | 6             | 0           | 2.918428 | -0.03461 | 2.987232 |
| 5             | 6             | 0           | 4.235735 | -0.53033 | 2.995171 |
| 6             | 6             | 0           | 4.631055 | -1.49707 | 3.924046 |
| 7             | 1             | 0           | 4.013721 | -2.73288 | 5.587305 |
| 8             | 1             | 0           | 1.680483 | -1.86895 | 5.59378  |
| 9             | 1             | 0           | 5.65052  | -1.86989 | 3.918311 |
| 10            | 6             | 0           | -2.79136 | 0.393124 | 4.881783 |
| 11            | 6             | 0           | -4.10633 | 0.867223 | 4.883666 |
| 12            | 6             | 0           | -4.50289 | 1.83437  | 3.947731 |
| 13            | 6             | 0           | -3.58221 | 2.321382 | 3.015616 |
| 14            | 6             | 0           | -2.2552  | 1.852627 | 3.000519 |
| 15            | 6             | 0           | -1.85338 | 0.873192 | 3.948654 |
| 16            | 1             | 0           | -2.47698 | -0.35327 | 5.603611 |
| 17            | 1             | 0           | -4.81866 | 0.487865 | 5.609602 |
| 18            | 1             | 0           | -5.52296 | 2.205548 | 3.94734  |
| 19            | 1             | 0           | -3.88124 | 3.070563 | 2.290159 |
| 20            | 6             | 0           | 1.765    | 2.783521 | 0.263258 |
| 21            | 6             | 0           | 0.429843 | 3.270551 | 0.266847 |
| 22            | 6             | 0           | 0.04838  | 4.239763 | -0.67972 |
| 23            | 6             | 0           | 0.964614 | 4.723524 | -1.61797 |
| 24            | 6             | 0           | 2.282758 | 4.242574 | -1.62151 |
| 25            | 6             | 0           | 2.676478 | 3.2809   | -0.68679 |
| 26            | 1             | 0           | -0.97191 | 4.60835  | -0.66976 |
| 27            | 1             | 0           | 0.655994 | 5.471345 | -2.34176 |
| 28            | 1             | 0           | 2.997046 | 4.617174 | -2.34799 |
| 29            | 6             | 0           | 2.529374 | 0.957501 | 2.028524 |
| 30            | 6             | 0           | 0.63657  | -0.04089 | 3.958318 |
| 31            | 6             | 0           | -0.50864 | 0.376958 | 3.960783 |
| 32            | 6             | 0           | -1.32328 | 2.363332 | 2.038542 |
| 33            | 6             | 0           | 2.185404 | 1.798263 | 1.21567  |
| 34            | 6             | 0           | -0.52176 | 2.785887 | 1.223092 |
| 35            | 47            | 0           | -0.03359 | 0.454152 | 2.246995 |
| 36            | 6             | 0           | 4.121457 | 2.748367 | -0.68031 |
| 37            | 6             | 0           | 5.248541 | 2.332991 | -0.67525 |
| 38            | 6             | 0           | 5.240227 | 0.011504 | 1.961244 |
| 39            | 6             | 0           | 6.023723 | 0.434131 | 1.154777 |
| 40            | 6             | 0           | 6.693519 | 1.800452 | -0.66877 |
| 41            | 6             | 0           | 7.672983 | 2.431379 | -1.43545 |
| 42            | 6             | 0           | 7.022865 | 0.686245 | 0.104071 |



|    |   |   |          |          |          |
|----|---|---|----------|----------|----------|
| 43 | 6 | 0 | 8.982208 | 1.949339 | -1.42889 |
| 44 | 1 | 0 | 7.413838 | 3.309683 | -2.04427 |
| 45 | 6 | 0 | 8.331672 | 0.204054 | 0.110183 |
| 46 | 6 | 0 | 9.311536 | 0.835889 | -0.65603 |
| 47 | 1 | 0 | 9.754377 | 2.447179 | -2.03308 |
| 48 | 1 | 0 | 8.591537 | -0.67407 | 0.719142 |
| 49 | 1 | 0 | 10.34332 | 0.455728 | -0.65088 |

**2GY@Ag<sub>side</sub>**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.709412 | -1.98299 | 4.863836 |
| 2             | 6             | 0           | 2.398041 | -1.4992  | 4.868987 |
| 3             | 6             | 0           | 1.984953 | -0.52682 | 3.939172 |
| 4             | 6             | 0           | 2.918428 | -0.03461 | 2.987232 |
| 5             | 6             | 0           | 4.235735 | -0.53033 | 2.995171 |
| 6             | 6             | 0           | 4.631055 | -1.49707 | 3.924046 |
| 7             | 1             | 0           | 4.013721 | -2.73288 | 5.587305 |
| 8             | 1             | 0           | 1.680483 | -1.86895 | 5.59378  |
| 9             | 1             | 0           | 5.65052  | -1.86989 | 3.918311 |
| 10            | 6             | 0           | -2.79136 | 0.393124 | 4.881783 |
| 11            | 6             | 0           | -4.10633 | 0.867223 | 4.883666 |
| 12            | 6             | 0           | -4.50289 | 1.83437  | 3.947731 |
| 13            | 6             | 0           | -3.58221 | 2.321382 | 3.015616 |
| 14            | 6             | 0           | -2.2552  | 1.852627 | 3.000519 |
| 15            | 6             | 0           | -1.85338 | 0.873192 | 3.948654 |
| 16            | 1             | 0           | -2.47698 | -0.35327 | 5.603611 |
| 17            | 1             | 0           | -4.81866 | 0.487865 | 5.609602 |
| 18            | 1             | 0           | -5.52296 | 2.205548 | 3.94734  |
| 19            | 1             | 0           | -3.88124 | 3.070563 | 2.290159 |
| 20            | 6             | 0           | 1.765    | 2.783521 | 0.263258 |
| 21            | 6             | 0           | 0.429843 | 3.270551 | 0.266847 |
| 22            | 6             | 0           | 0.04838  | 4.239763 | -0.67972 |
| 23            | 6             | 0           | 0.964614 | 4.723524 | -1.61797 |
| 24            | 6             | 0           | 2.282758 | 4.242574 | -1.62151 |
| 25            | 6             | 0           | 2.676478 | 3.2809   | -0.68679 |
| 26            | 1             | 0           | -0.97191 | 4.60835  | -0.66976 |
| 27            | 1             | 0           | 0.655994 | 5.471345 | -2.34176 |
| 28            | 1             | 0           | 2.997046 | 4.617174 | -2.34799 |
| 29            | 6             | 0           | 2.529374 | 0.957501 | 2.028524 |
| 30            | 6             | 0           | 0.63657  | -0.04089 | 3.958318 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 31 | 6  | 0 | -0.50864 | 0.376958 | 3.960783 |
| 32 | 6  | 0 | -1.32328 | 2.363332 | 2.038542 |
| 33 | 6  | 0 | 2.185404 | 1.798263 | 1.21567  |
| 34 | 6  | 0 | -0.52176 | 2.785887 | 1.223092 |
| 35 | 47 | 0 | -3.47599 | 0.398029 | 3.215293 |
| 36 | 6  | 0 | 4.121457 | 2.748367 | -0.68031 |
| 37 | 6  | 0 | 5.248541 | 2.332991 | -0.67525 |
| 38 | 6  | 0 | 5.240227 | 0.011504 | 1.961244 |
| 39 | 6  | 0 | 6.023723 | 0.434131 | 1.154777 |
| 40 | 6  | 0 | 6.693519 | 1.800452 | -0.66877 |
| 41 | 6  | 0 | 7.672983 | 2.431379 | -1.43545 |
| 42 | 6  | 0 | 7.022865 | 0.686245 | 0.104071 |
| 43 | 6  | 0 | 8.982208 | 1.949339 | -1.42889 |
| 44 | 1  | 0 | 7.413838 | 3.309683 | -2.04427 |
| 45 | 6  | 0 | 8.331672 | 0.204054 | 0.110183 |
| 46 | 6  | 0 | 9.311536 | 0.835889 | -0.65603 |
| 47 | 1  | 0 | 9.754377 | 2.447179 | -2.03308 |
| 48 | 1  | 0 | 8.591537 | -0.67407 | 0.719142 |
| 49 | 1  | 0 | 10.34332 | 0.455728 | -0.65088 |

**2GY@2Ag<sub>perpendicular</sub>**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.709412 | -1.98299 | 4.863836 |
| 2             | 6             | 0           | 2.398041 | -1.4992  | 4.868987 |
| 3             | 6             | 0           | 1.984953 | -0.52682 | 3.939172 |
| 4             | 6             | 0           | 2.918428 | -0.03461 | 2.987232 |
| 5             | 6             | 0           | 4.235735 | -0.53033 | 2.995171 |
| 6             | 6             | 0           | 4.631055 | -1.49707 | 3.924046 |
| 7             | 1             | 0           | 4.013721 | -2.73288 | 5.587305 |
| 8             | 1             | 0           | 1.680483 | -1.86895 | 5.59378  |
| 9             | 1             | 0           | 5.65052  | -1.86989 | 3.918311 |
| 10            | 6             | 0           | -2.79136 | 0.393124 | 4.881783 |
| 11            | 6             | 0           | -4.10633 | 0.867223 | 4.883666 |
| 12            | 6             | 0           | -4.50289 | 1.83437  | 3.947731 |
| 13            | 6             | 0           | -3.58221 | 2.321382 | 3.015616 |
| 14            | 6             | 0           | -2.2552  | 1.852627 | 3.000519 |
| 15            | 6             | 0           | -1.85338 | 0.873192 | 3.948654 |
| 16            | 1             | 0           | -2.47698 | -0.35327 | 5.603611 |
| 17            | 1             | 0           | -4.81866 | 0.487865 | 5.609602 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 18 | 1  | 0 | -5.52296 | 2.205548 | 3.94734  |
| 19 | 1  | 0 | -3.88124 | 3.070563 | 2.290159 |
| 20 | 6  | 0 | 1.765    | 2.783521 | 0.263258 |
| 21 | 6  | 0 | 0.429843 | 3.270551 | 0.266847 |
| 22 | 6  | 0 | 0.04838  | 4.239763 | -0.67972 |
| 23 | 6  | 0 | 0.964614 | 4.723524 | -1.61797 |
| 24 | 6  | 0 | 2.282758 | 4.242574 | -1.62151 |
| 25 | 6  | 0 | 2.676478 | 3.2809   | -0.68679 |
| 26 | 1  | 0 | -0.97191 | 4.60835  | -0.66976 |
| 27 | 1  | 0 | 0.655994 | 5.471345 | -2.34176 |
| 28 | 1  | 0 | 2.997046 | 4.617174 | -2.34799 |
| 29 | 6  | 0 | 2.529374 | 0.957501 | 2.028524 |
| 30 | 6  | 0 | 0.63657  | -0.04089 | 3.958318 |
| 31 | 6  | 0 | -0.50864 | 0.376958 | 3.960783 |
| 32 | 6  | 0 | -1.32328 | 2.363332 | 2.038542 |
| 33 | 6  | 0 | 2.185404 | 1.798263 | 1.21567  |
| 34 | 6  | 0 | -0.52176 | 2.785887 | 1.223092 |
| 35 | 47 | 0 | -0.07575 | 0.207012 | 1.684948 |
| 36 | 6  | 0 | 4.121457 | 2.748367 | -0.68031 |
| 37 | 6  | 0 | 5.248541 | 2.332991 | -0.67525 |
| 38 | 6  | 0 | 5.240227 | 0.011504 | 1.961244 |
| 39 | 6  | 0 | 6.023723 | 0.434131 | 1.154777 |
| 40 | 6  | 0 | 6.693519 | 1.800452 | -0.66877 |
| 41 | 6  | 0 | 7.672983 | 2.431379 | -1.43545 |
| 42 | 6  | 0 | 7.022865 | 0.686245 | 0.104071 |
| 43 | 6  | 0 | 8.982208 | 1.949339 | -1.42889 |
| 44 | 1  | 0 | 7.413838 | 3.309683 | -2.04427 |
| 45 | 6  | 0 | 8.331672 | 0.204054 | 0.110183 |
| 46 | 6  | 0 | 9.311536 | 0.835889 | -0.65603 |
| 47 | 1  | 0 | 9.754377 | 2.447179 | -2.03308 |
| 48 | 1  | 0 | 8.591537 | -0.67407 | 0.719142 |
| 49 | 1  | 0 | 10.34332 | 0.455728 | -0.65088 |
| 50 | 47 | 0 | 0.364254 | 1.972849 | 3.429411 |

**2GY@2Ag<sub>above</sub>**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.709412 | -1.98299 | 4.863836 |
| 2             | 6             | 0           | 2.398041 | -1.4992  | 4.868987 |
| 3             | 6             | 0           | 1.984953 | -0.52682 | 3.939172 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 4  | 6  | 0 | 2.918428 | -0.03461 | 2.987232 |
| 5  | 6  | 0 | 4.235735 | -0.53033 | 2.995171 |
| 6  | 6  | 0 | 4.631055 | -1.49707 | 3.924046 |
| 7  | 1  | 0 | 4.013721 | -2.73288 | 5.587305 |
| 8  | 1  | 0 | 1.680483 | -1.86895 | 5.59378  |
| 9  | 1  | 0 | 5.65052  | -1.86989 | 3.918311 |
| 10 | 6  | 0 | -2.79136 | 0.393124 | 4.881783 |
| 11 | 6  | 0 | -4.10633 | 0.867223 | 4.883666 |
| 12 | 6  | 0 | -4.50289 | 1.83437  | 3.947731 |
| 13 | 6  | 0 | -3.58221 | 2.321382 | 3.015616 |
| 14 | 6  | 0 | -2.2552  | 1.852627 | 3.000519 |
| 15 | 6  | 0 | -1.85338 | 0.873192 | 3.948654 |
| 16 | 1  | 0 | -2.47698 | -0.35327 | 5.603611 |
| 17 | 1  | 0 | -4.81866 | 0.487865 | 5.609602 |
| 18 | 1  | 0 | -5.52296 | 2.205548 | 3.94734  |
| 19 | 1  | 0 | -3.88124 | 3.070563 | 2.290159 |
| 20 | 6  | 0 | 1.765    | 2.783521 | 0.263258 |
| 21 | 6  | 0 | 0.429843 | 3.270551 | 0.266847 |
| 22 | 6  | 0 | 0.04838  | 4.239763 | -0.67972 |
| 23 | 6  | 0 | 0.964614 | 4.723524 | -1.61797 |
| 24 | 6  | 0 | 2.282758 | 4.242574 | -1.62151 |
| 25 | 6  | 0 | 2.676478 | 3.2809   | -0.68679 |
| 26 | 1  | 0 | -0.97191 | 4.60835  | -0.66976 |
| 27 | 1  | 0 | 0.655994 | 5.471345 | -2.34176 |
| 28 | 1  | 0 | 2.997046 | 4.617174 | -2.34799 |
| 29 | 6  | 0 | 2.529374 | 0.957501 | 2.028524 |
| 30 | 6  | 0 | 0.63657  | -0.04089 | 3.958318 |
| 31 | 6  | 0 | -0.50864 | 0.376958 | 3.960783 |
| 32 | 6  | 0 | -1.32328 | 2.363332 | 2.038542 |
| 33 | 6  | 0 | 2.185404 | 1.798263 | 1.21567  |
| 34 | 6  | 0 | -0.52176 | 2.785887 | 1.223092 |
| 35 | 47 | 0 | -1.07285 | -0.02162 | 1.890424 |
| 36 | 6  | 0 | 4.121457 | 2.748367 | -0.68031 |
| 37 | 6  | 0 | 5.248541 | 2.332991 | -0.67525 |
| 38 | 6  | 0 | 5.240227 | 0.011504 | 1.961244 |
| 39 | 6  | 0 | 6.023723 | 0.434131 | 1.154777 |
| 40 | 6  | 0 | 6.693519 | 1.800452 | -0.66877 |
| 41 | 6  | 0 | 7.672983 | 2.431379 | -1.43545 |
| 42 | 6  | 0 | 7.022865 | 0.686245 | 0.104071 |
| 43 | 6  | 0 | 8.982208 | 1.949339 | -1.42889 |
| 44 | 1  | 0 | 7.413838 | 3.309683 | -2.04427 |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 45 | 6  | 0 | 8.331672 | 0.204054 | 0.110183 |
| 46 | 6  | 0 | 9.311536 | 0.835889 | -0.65603 |
| 47 | 1  | 0 | 9.754377 | 2.447179 | -2.03308 |
| 48 | 1  | 0 | 8.591537 | -0.67407 | 0.719142 |
| 49 | 1  | 0 | 10.34332 | 0.455728 | -0.65088 |
| 50 | 47 | 0 | 1.246065 | 0.063347 | 0.927066 |

**2GY@3Ag<sub>center</sub>**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | -0.95305 | -4.40895 | -1.77083 |
| 2             | 6             | 0           | 0.215386 | -3.64336 | -1.81992 |
| 3             | 6             | 0           | 0.183676 | -2.26202 | -1.55233 |
| 4             | 6             | 0           | -1.0553  | -1.64475 | -1.23022 |
| 5             | 6             | 0           | -2.22365 | -2.42839 | -1.18592 |
| 6             | 6             | 0           | -2.17629 | -3.79959 | -1.45284 |
| 7             | 1             | 0           | -0.91321 | -5.4734  | -1.97984 |
| 8             | 1             | 0           | 1.164445 | -4.10731 | -2.06682 |
| 9             | 1             | 0           | -3.08563 | -4.39122 | -1.41515 |
| 10            | 6             | 0           | 4.83997  | -0.62784 | -1.99551 |
| 11            | 6             | 0           | 6.012162 | 0.132591 | -2.03583 |
| 12            | 6             | 0           | 5.963753 | 1.508076 | -1.76325 |
| 13            | 6             | 0           | 4.743607 | 2.114678 | -1.45188 |
| 14            | 6             | 0           | 3.555286 | 1.361873 | -1.40608 |
| 15            | 6             | 0           | 3.604191 | -0.03131 | -1.68242 |
| 16            | 1             | 0           | 4.869321 | -1.69151 | -2.20695 |
| 17            | 1             | 0           | 6.958002 | -0.34124 | -2.27911 |
| 18            | 1             | 0           | 6.872029 | 2.101674 | -1.79497 |
| 19            | 1             | 0           | 4.698295 | 3.178064 | -1.24179 |
| 20            | 6             | 0           | -1.19734 | 2.360985 | -0.43889 |
| 21            | 6             | 0           | -0.00744 | 3.136815 | -0.48439 |
| 22            | 6             | 0           | -0.07359 | 4.51507  | -0.20708 |
| 23            | 6             | 0           | -1.29097 | 5.123445 | 0.111846 |
| 24            | 6             | 0           | -2.46569 | 4.357396 | 0.15684  |
| 25            | 6             | 0           | -2.41575 | 2.987783 | -0.11738 |
| 26            | 1             | 0           | 0.838409 | 5.101347 | -0.24562 |
| 27            | 1             | 0           | -1.32655 | 6.187622 | 0.323045 |
| 28            | 1             | 0           | -3.41287 | 4.827084 | 0.402911 |
| 29            | 6             | 0           | -1.12125 | -0.23955 | -0.95482 |
| 30            | 6             | 0           | 1.390938 | -1.49123 | -1.6074  |

|    |    |   |          |          |          |
|----|----|---|----------|----------|----------|
| 31 | 6  | 0 | 2.41136  | -0.82537 | -1.646   |
| 32 | 6  | 0 | 2.312102 | 1.999702 | -1.08614 |
| 33 | 6  | 0 | -1.16381 | 0.95557  | -0.71861 |
| 34 | 6  | 0 | 1.248866 | 2.528668 | -0.81107 |
| 35 | 6  | 0 | -3.6996  | 2.138433 | -0.07338 |
| 36 | 6  | 0 | -4.701   | 1.475939 | -0.03906 |
| 37 | 6  | 0 | -3.56153 | -1.74941 | -0.83854 |
| 38 | 6  | 0 | -4.60506 | -1.2198  | -0.56757 |
| 39 | 6  | 0 | -5.98485 | 0.626588 | 0.004958 |
| 40 | 6  | 0 | -7.2302  | 1.248587 | 0.091237 |
| 41 | 6  | 0 | -5.90215 | -0.76562 | -0.04116 |
| 42 | 6  | 0 | -8.39329 | 0.479058 | 0.130294 |
| 43 | 1  | 0 | -7.29572 | 2.345696 | 0.127192 |
| 44 | 6  | 0 | -7.06496 | -1.53492 | -0.00158 |
| 45 | 6  | 0 | -8.31067 | -0.91255 | 0.083726 |
| 46 | 1  | 0 | -9.37507 | 0.969657 | 0.197876 |
| 47 | 1  | 0 | -7.0001  | -2.63216 | -0.03788 |
| 48 | 1  | 0 | -9.22725 | -1.51921 | 0.114678 |
| 49 | 47 | 0 | 2.982175 | -0.12651 | 0.485709 |
| 50 | 47 | 0 | 0.337096 | -0.33426 | 0.863595 |
| 51 | 47 | 0 | 2.019725 | -1.09997 | 2.533879 |

## 2GY

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.709412 | -1.98299 | 4.863836 |
| 2             | 6             | 0           | 2.398041 | -1.4992  | 4.868987 |
| 3             | 6             | 0           | 1.984953 | -0.52682 | 3.939172 |
| 4             | 6             | 0           | 2.918428 | -0.03461 | 2.987232 |
| 5             | 6             | 0           | 4.235735 | -0.53033 | 2.995171 |
| 6             | 6             | 0           | 4.631055 | -1.49707 | 3.924046 |
| 7             | 1             | 0           | 4.013721 | -2.73288 | 5.587305 |
| 8             | 1             | 0           | 1.680483 | -1.86895 | 5.59378  |
| 9             | 1             | 0           | 5.65052  | -1.86989 | 3.918311 |
| 10            | 6             | 0           | -2.79136 | 0.393124 | 4.881783 |
| 11            | 6             | 0           | -4.10633 | 0.867223 | 4.883666 |
| 12            | 6             | 0           | -4.50289 | 1.83437  | 3.947731 |
| 13            | 6             | 0           | -3.58221 | 2.321382 | 3.015616 |
| 14            | 6             | 0           | -2.2552  | 1.852627 | 3.000519 |
| 15            | 6             | 0           | -1.85338 | 0.873192 | 3.948654 |

|    |   |   |          |          |          |
|----|---|---|----------|----------|----------|
| 16 | 1 | 0 | -2.47698 | -0.35327 | 5.603611 |
| 17 | 1 | 0 | -4.81866 | 0.487865 | 5.609602 |
| 18 | 1 | 0 | -5.52296 | 2.205548 | 3.94734  |
| 19 | 1 | 0 | -3.88124 | 3.070563 | 2.290159 |
| 20 | 6 | 0 | 1.765    | 2.783521 | 0.263258 |
| 21 | 6 | 0 | 0.429843 | 3.270551 | 0.266847 |
| 22 | 6 | 0 | 0.04838  | 4.239763 | -0.67972 |
| 23 | 6 | 0 | 0.964614 | 4.723524 | -1.61797 |
| 24 | 6 | 0 | 2.282758 | 4.242574 | -1.62151 |
| 25 | 6 | 0 | 2.676478 | 3.2809   | -0.68679 |
| 26 | 1 | 0 | -0.97191 | 4.60835  | -0.66976 |
| 27 | 1 | 0 | 0.655994 | 5.471345 | -2.34176 |
| 28 | 1 | 0 | 2.997046 | 4.617174 | -2.34799 |
| 29 | 6 | 0 | 2.529374 | 0.957501 | 2.028524 |
| 30 | 6 | 0 | 0.63657  | -0.04089 | 3.958318 |
| 31 | 6 | 0 | -0.50864 | 0.376958 | 3.960783 |
| 32 | 6 | 0 | -1.32328 | 2.363332 | 2.038542 |
| 33 | 6 | 0 | 2.185404 | 1.798263 | 1.21567  |
| 34 | 6 | 0 | -0.52176 | 2.785887 | 1.223092 |
| 35 | 6 | 0 | 4.121457 | 2.748367 | -0.68031 |
| 36 | 6 | 0 | 5.248541 | 2.332991 | -0.67525 |
| 37 | 6 | 0 | 5.240227 | 0.011504 | 1.961244 |
| 38 | 6 | 0 | 6.023723 | 0.434131 | 1.154777 |
| 39 | 6 | 0 | 6.693519 | 1.800452 | -0.66877 |
| 40 | 6 | 0 | 7.672983 | 2.431379 | -1.43545 |
| 41 | 6 | 0 | 7.022865 | 0.686245 | 0.104071 |
| 42 | 6 | 0 | 8.982208 | 1.949339 | -1.42889 |
| 43 | 1 | 0 | 7.413838 | 3.309683 | -2.04427 |
| 44 | 6 | 0 | 8.331672 | 0.204054 | 0.110183 |
| 45 | 6 | 0 | 9.311536 | 0.835889 | -0.65603 |
| 46 | 1 | 0 | 9.754377 | 2.447179 | -2.03308 |
| 47 | 1 | 0 | 8.591537 | -0.67407 | 0.719142 |
| 48 | 1 | 0 | 10.34332 | 0.455728 | -0.65088 |