Electronic Supplementary Material (ESI) for Faraday Discussions.


# Characterization of Pt-doping effects on nanoparticle emission: A theoretical look at $Au_{24}Pt(SH)_{18}$ and $Au_{24}Pt(SC_3H_7)_{18}$

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## Supporting Information

**Table S1.** Relative energies of $Au_{24}Pt(SC_3H_7)_{18}$ isomers for different locations of the dopant. One BP86/TZP calculation was performed to check the relative energies in each location (center, outer shell of the core, staple).

| Dopant Position | | Relative Energy (eV) | |
|---|---|---|---|
| Atom # | Location | BP86/DZ | BP86/TZP |
| P1 | Center | 0.00 | 0.00 |
| P4 | Core (Outer Shell) | 0.38 | -- |
| P5 | Core (Outer Shell) | 0.26 | 0.03 |
| P7 | Core (Outer Shell) | 0.53 | -- |
| P14 | Core (Outer Shell) | 0.63 | -- |
| P15 | Core (Outer Shell) | 0.53 | -- |
| P22 | Core (Outer Shell) | 0.28 | -- |
| P24 | Staple Motif | 0.69 | 0.30 |

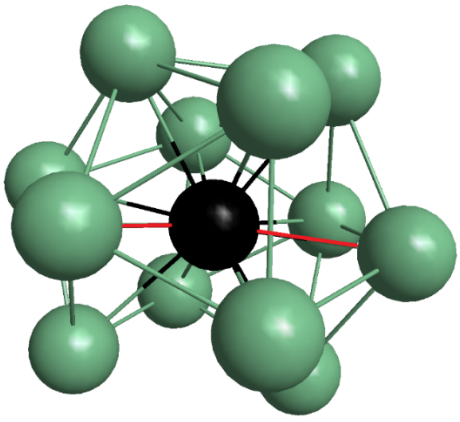

**Figure S1.** Illustration of the flattened oblate $Au_{12}Pt$ core as it appears in the optimized BP86/DZ ground state of $Au_{24}Pt(SC_3H_7)_{18}$. The two bonds that are ~0.11 Å larger than the rest of the Au core – Pt center bonds are colored in red.

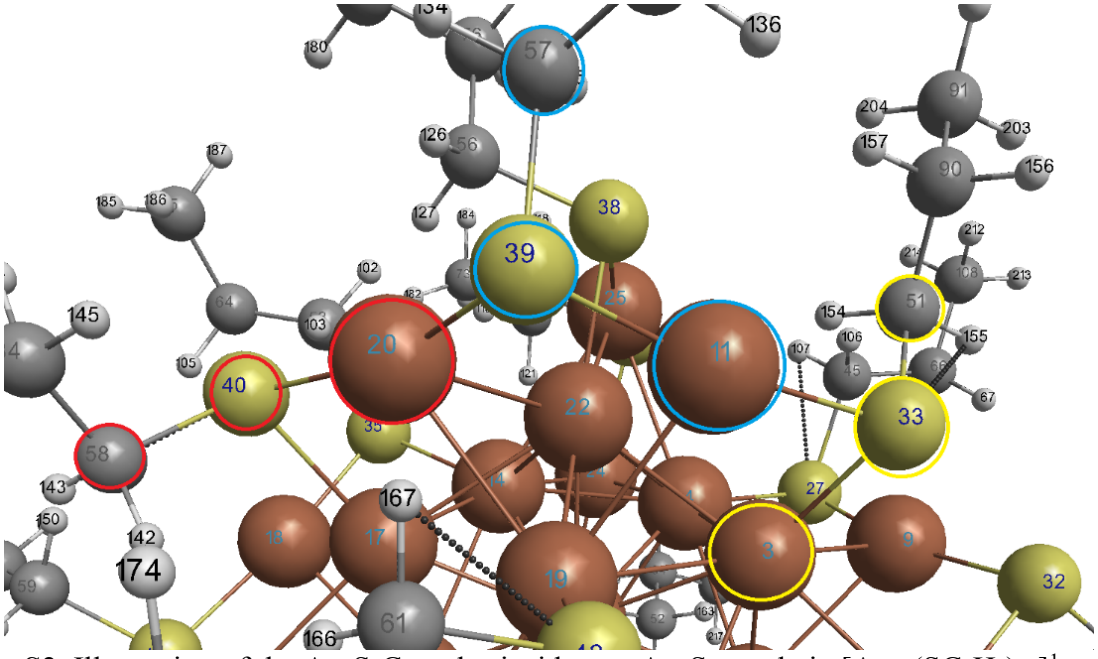


**Figure S2.** Illustration of the Au-S-C angles inside one $Au_2S_3$ staple in $[Au_{25}(SC_3H_7)_{18}]^{1-}$ outlined by the red, blue, and yellow circles. The S-C connection in red is directionally opposite from the S-C in blue, creating a trans configuration. The S-C connection in yellow is directionally the same as the one in blue, creating a cis configuration. Altogether, this forms an alternating trans/cis configuration across the staples. Further, the anti configuration of the propyl groups can be seen in the propyl group connected to sulfur atom 33.

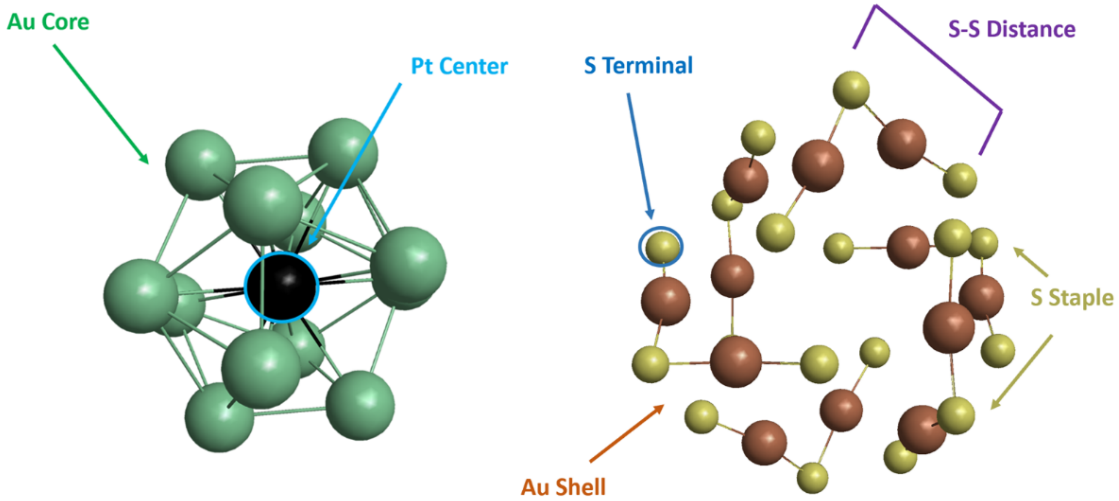


**Figure S3.** Atom labels for bond distance analysis shown in table 1.

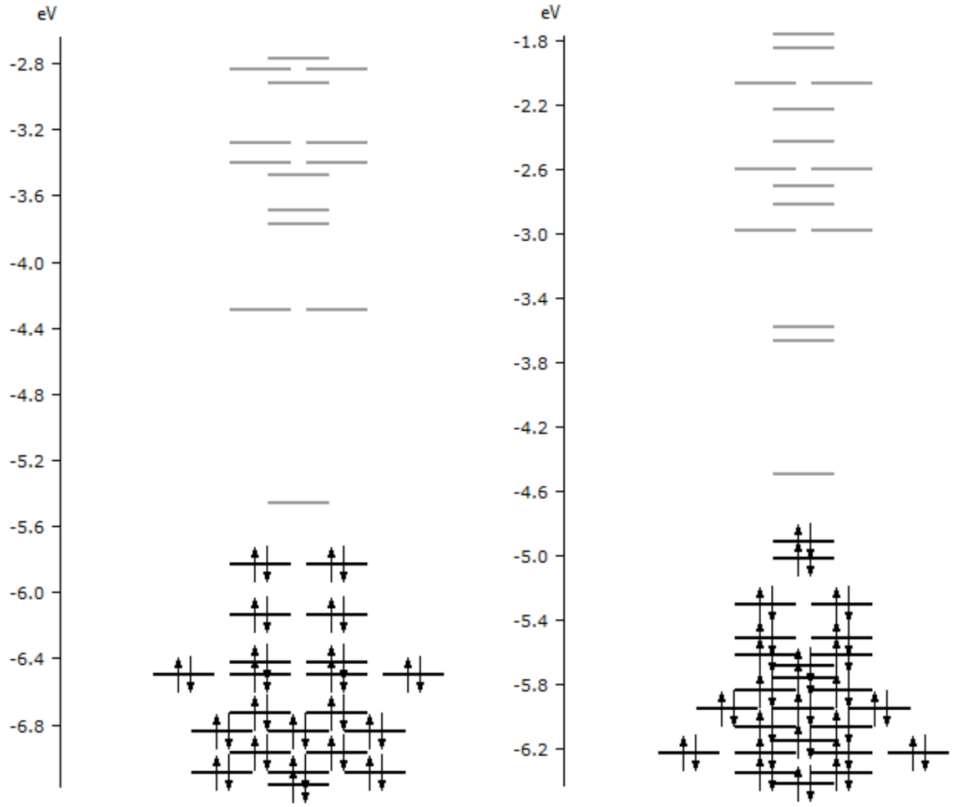


**Figure S4.** BP86/DZ molecular orbital diagram in eV for $Au_{24}Pt(SR)_{18}$ for R = H (left) and R = $C_3H_7$ (right).

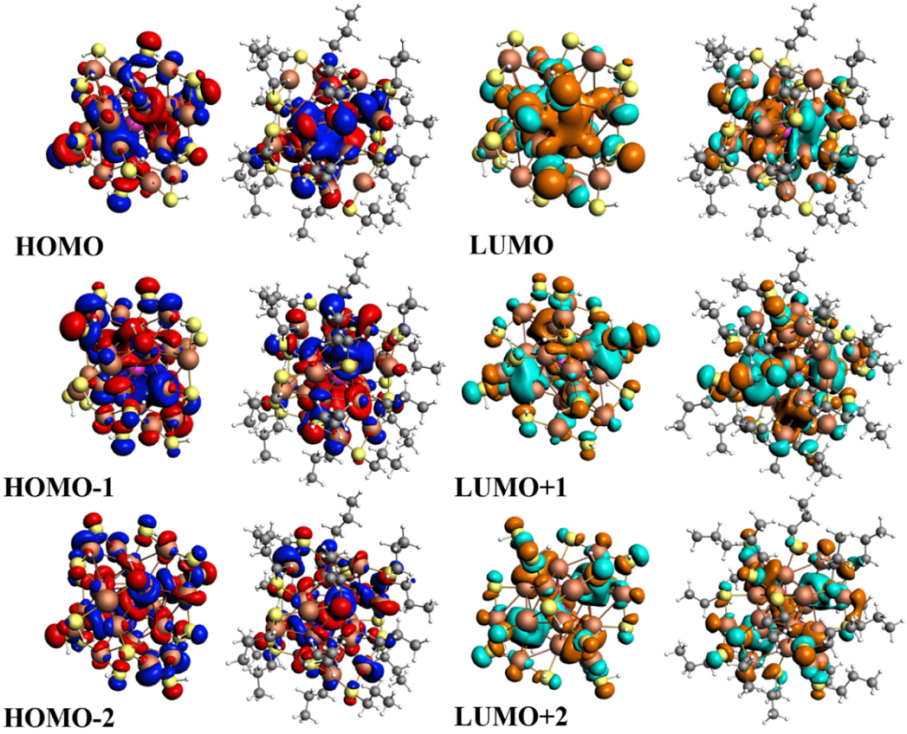


**Figure S5.** Images of the first six frontier MOs (H-2 through L+2) for $Au_{24}Pt(SR)_{18}$ for R = H (left), and R = $C_3H_7$ (right).

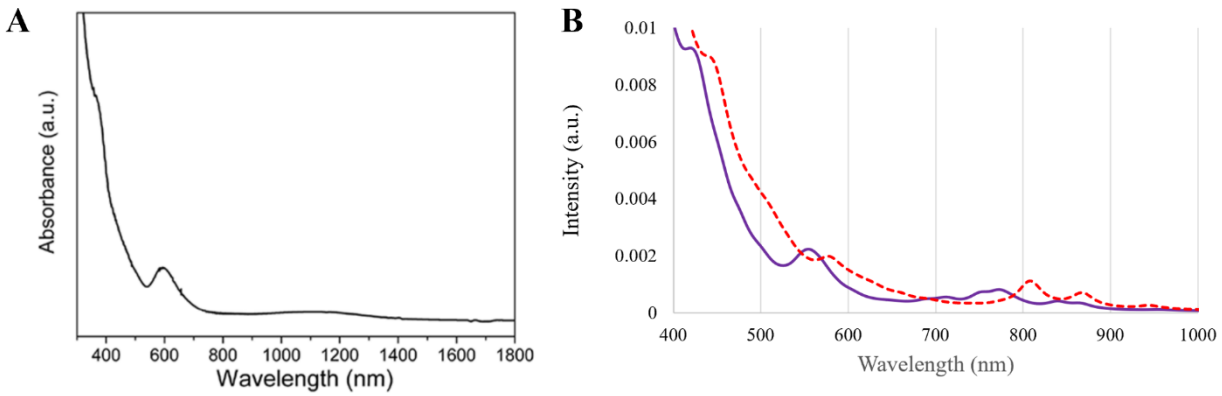


**Figure S6.** Absorption spectrum of $Au_{24}Pt(SR)_{18}$ clusters. (A) Experimental results reprinted with permission from JACS 2008, 130, 5883-5885. Copyright 2008 American Chemical Society. (B) Theoretical spectrum calculated with TDDFT+TB* at the BP86/DZ level of theory for R=H (solid purple) and R=$C_3H_7$ (dotted red).

*Note: The hydrogen results completed with TDDFT only included 100 vertical excitations. To achieve higher energy ranges at a cheaper computational cost, time-dependent density-functional theory plus tight binding (TDDFT+TB) (Ref. 1) was used to calculate the first 1500 vertical excitation energies. These energies were then fit with a 30 nm FWHM.

**Table S2.** Absorption details (state, energy, transition type) of $Au_{24}Pt(SR)_{18}$ when R = H (left), and R = $C_3H_7$ (right)

| **$PtAu_{24}(SH)_{18}^0$** TDDFT | | | **$PtAu_{24}(SC_3H_7)_{18}^0$** TDDFT | | |
|---|---|---|---|---|---|
| State | Energy (eV) | Major transitions | State | Energy (eV) | Major transitions |
| $S_1$ | 0.423 | P→P | $S_1$ | 0.473 | P→P |
| $S_2$ | 0.454 | | $S_2$ | 0.585 | |
| $S_3$ | 0.739 | d→P | $S_3$ | 0.875 | d→P |
| $S_4$ | 0.796 | | $S_4$ | 0.941 | |
| $S_5$ | 1.000 | | $S_5$ | 1.087 | |
| $S_6$ | 1.023 | | $S_6$ | 1.131 | |
| $S_7$ | 1.081 | | $S_7$ | 1.157 | |
| $S_8$ | 1.088 | | $S_8$ | 1.205 | |
| $S_9$ | 1.095 | | $S_9$ | 1.232 | |
| $S_{10}$ | 1.112 | | $S_{10}$ | 1.297 | |
| $S_{11}$ | 1.318 | | $S_{11}$ | 1.326 | P→D |
| $S_{12}$ | 1.366 | | $S_{12}$ | 1.365 | |
| $S_{13}$ | 1.446 | | $S_{13}$ | 1.407 | d →P |
| $S_{14}$ | 1.476 | | $S_{14}$ | 1.434 | P→D |
| $S_{15}$ | 1.494 | | $S_{15}$ | 1.455 | d→ P |
| $S_{16}$ | 1.563 | P→D | $S_{16}$ | 1.500 | |
| $S_{17}$ | 1.578 | d→P | $S_{17}$ | 1.543 | d→P and P→D mixed |
| $S_{18}$ | 1.580 | d→P and P→D mixed | $S_{18}$ | 1.548 | |
| $S_{19}$ | 1.598 | | $S_{19}$ | 1.551 | d→P |
| $S_{20}$ | 1.615 | | $S_{20}$ | 1.614 | |
| $S_{21}$ | 1.661 | P→D | $S_{21}$ | 1.654 | |

**Table S3.** Average bond distances (Å) and standard deviation of the core and shell atoms at the BP86/DZ $S_0$, $S_3$, $S_{15}$, $S_{18}$ and $S_{21}$ minima.

| State | Ligand | Pt Center – Au Core | Au Core- Au Core | Au Core – Au Shell | Au Core – S Terminal | Au Shell – S Staple | S-S Distance |
|---|---|---|---|---|---|---|---|
| **$S_0$** | **R = Propyl** | **2.853** | **3.003** | **3.133** | **2.523** | **2.424** | **4.817** |
| | SD | 0.054 | 0.256 | 0.157 | 0.030 | 0.008 | 0.009 |
| $S_3$ | R = Propyl | **2.822** | **2.971** | **3.112** | **2.530** | **2.427** | **4.820** |
| | SD | 0.029 | 0.150 | 0.115 | 0.019 | 0.008 | 0.011 |
| $S_{19}$ | R = Propyl | 2.848 | 2.999 | 3.126 | 2.528 | 2.429 | 4.819 |
| | SD | 0.043 | 0.221 | 0.165 | 0.025 | 0.011 | 0.010 |
| **$S_0$** | **R = Hydrogen** | **2.827** | **2.974** | **3.115** | **2.516** | **2.422** | **4.809** |
| | SD | 0.016 | 0.189 | 0.119 | 0.023 | 0.005 | 0.006 |
| $S_{15}$ | R = Hydrogen | **2.816** | **2.963** | **3.109** | **2.531** | **2.425** | **4.806** |
| | SD | 0.017 | 0.126 | 0.107 | 0.008 | 0.005 | 0.005 |
| $S_{18}$ | R = Hydrogen | **2.808** | **2.954** | **3.095** | **2.532** | **2.430** | **4.815** |
| | SD | 0.015 | 0.108 | 0.105 | 0.006 | 0.008 | 0.009 |
| $S_{21}$ | R = Hydrogen | **2.830** | **2.978** | **3.116** | **2.521** | **2.426** | **4.810** |
| | SD | 0.014 | 0.182 | 0.137 | 0.015 | 0.006 | 0.006 |

**Reference**

[1] R. Rüger, E. van Lenthe, T. Heine, L. Visscher. Tight-binding approximations to time-dependent density functional theory — A fast approach for the calculation of electronically excited states. *The Journal of Chemical Physics.* 2016, **144,** 184103.

**Coordinates in angstroms:**

**$Au_{24}Pt(SH)_{18}$ $S_0$**

| | | | |
|---|---|---|---|
| Pt | -0.002185 | 0.003993 | 0.003993 |
| Au | -2.121659 | 1.527578 | -1.075045 |
| Au | -2.536522 | -1.243027 | -0.255114 |
| Au | 0.057064 | -2.833653 | -0.242455 |
| Au | -0.779807 | -1.188514 | -2.410874 |
| Au | -3.656018 | -0.571270 | -3.008225 |
| Au | 2.033871 | -1.004752 | -1.692732 |
| Au | 1.621753 | -0.179875 | -4.557285 |
| Au | -2.362065 | -3.782819 | -2.015529 |
| Au | 1.011730 | 1.546944 | -2.118314 |
| Au | -3.997343 | -1.573559 | 2.478594 |
| Au | -2.932138 | 3.841441 | 0.819628 |
| Au | -1.157848 | 4.158157 | -2.250192 |
| Au | 2.122935 | -1.516934 | 1.075095 |
| Au | 2.532880 | 1.254078 | 0.256705 |
| Au | -0.059766 | 2.843583 | 0.251232 |
| Au | 0.780535 | 1.192017 | 2.418290 |
| Au | 3.658581 | 0.574059 | 3.006310 |
| Au | -2.035384 | 1.022397 | 1.695393 |
| Au | -1.629064 | 0.197242 | 4.561886 |
| Au | 2.359104 | 3.789011 | 2.018716 |
| Au | -1.028545 | -1.539520 | 2.121018 |
| Au | 3.987215 | 1.586659 | -2.472205 |
| Au | 2.920723 | -3.837924 | -0.806508 |
| Au | 1.147722 | -4.134646 | 2.267729 |
| S | -3.871953 | 1.831066 | -2.825623 |
| S | -0.958106 | -5.142738 | -0.580704 |
| S | -2.674856 | 5.498743 | -0.930391 |
| S | 0.345807 | 3.187048 | -3.871071 |
| S | 3.619389 | 1.164837 | -4.824600 |
| S | -0.384065 | -1.498873 | -4.856860 |
| S | -3.954087 | -2.902172 | -3.613732 |
| S | -4.860795 | -2.110453 | 0.279872 |
| S | 3.660929 | -2.609508 | -2.770502 |
| S | 3.883951 | -1.826773 | 2.814940 |
| S | 0.951098 | 5.154018 | 0.591709 |
| S | 2.644144 | -5.492572 | 0.943214 |
| S | -0.342343 | -3.154532 | 3.893022 |
| S | -3.635547 | -1.137241 | 4.828462 |
| S | 0.388207 | 1.497341 | 4.865142 |
| S | 3.961125 | 2.905439 | 3.605202 |
| S | 4.859367 | 2.117278 | -0.274291 |
| S | -3.657643 | 2.618772 | 2.795025 |
| H | -3.032046 | 2.179841 | -3.881839 |

| | | | |
|---|---|---|---|
| H | -1.781436 | -5.107952 | 0.543297 |
| H | -3.844520 | 5.201044 | -1.628782 |
| H | -0.560976 | 2.372681 | -4.544938 |
| H | 2.971629 | 2.366297 | -5.113326 |
| H | 0.207397 | -2.759637 | -4.791901 |
| H | -3.126181 | -2.878920 | -4.735836 |
| H | -4.565167 | -3.472714 | 0.275165 |
| H | 2.785565 | -3.207564 | -3.675682 |
| H | 3.051228 | -2.185909 | 3.873514 |
| H | 1.774431 | 5.123803 | -0.532395 |
| H | 3.820693 | -5.213748 | 1.638038 |
| H | 0.565948 | -2.326250 | 4.547595 |
| H | -2.994039 | -2.339165 | 5.128994 |
| H | -0.190306 | 2.764186 | 4.803841 |
| H | 3.144894 | 2.888211 | 4.735817 |
| H | 4.568639 | 3.480513 | -0.267318 |
| H | -2.772629 | 3.217657 | 3.690208 |

**$Au_{24}Pt(SC_3H_7)_{18}$ $S_0$**

| | | | |
|---|---|---|---|
| Pt | -0.053679 | -0.006859 | -0.182174 |
| Au | -1.892125 | 1.649316 | -1.596362 |
| Au | -2.531068 | -1.300742 | -0.539691 |
| Au | -0.110181 | -2.807606 | -0.623852 |
| Au | -0.912940 | -0.846609 | -2.801564 |
| Au | -4.035386 | -0.550192 | -2.982782 |
| Au | 1.832322 | -1.055146 | -1.968961 |
| Au | 1.504130 | -0.471998 | -4.906116 |
| Au | -2.318773 | -3.483774 | -2.785123 |
| Au | 0.808355 | 1.483050 | -2.465084 |
| Au | -4.174445 | -1.015267 | 2.310488 |
| Au | -3.024566 | 3.894895 | 0.078691 |
| Au | -0.551589 | 4.397482 | -2.362764 |
| Au | 1.433881 | -1.808113 | 1.493940 |
| Au | 2.249244 | 1.664802 | 0.009306 |
| Au | -0.260904 | 2.883198 | 0.281999 |
| Au | 0.737673 | 0.924125 | 2.294980 |
| Au | 3.779592 | 0.742232 | 2.354535 |
| Au | -2.088493 | 1.024996 | 1.471048 |
| Au | -1.634977 | 0.308569 | 4.406045 |
| Au | 2.058472 | 3.727593 | 2.250787 |
| Au | -1.254772 | -1.554744 | 2.027238 |
| Au | 3.780629 | 1.125664 | -3.010792 |
| Au | 2.602691 | -3.975651 | -0.190633 |
| Au | 0.031477 | -4.483805 | 1.952955 |
| S | -3.997100 | 1.867143 | -2.911577 |
| S | -0.161879 | -4.547265 | -2.512087 |

| | | | |
|---|---|---|---|
| S | -2.232664 | 5.752257 | -1.258717 |
| S | 1.257239 | 3.586182 | -3.762600 |
| S | 3.927936 | -0.483727 | -4.826803 |
| S | -0.868980 | -0.684589 | -5.348418 |
| S | -4.632193 | -2.900712 | -3.205532 |
| S | -4.829003 | -1.983806 | 0.203598 |
| S | 3.893869 | -2.339444 | -1.406163 |
| S | 3.744196 | -1.677121 | 2.412511 |
| S | -0.105273 | 4.777111 | 2.006955 |
| S | 1.540816 | -5.951483 | 0.725099 |
| S | -1.528082 | -3.565331 | 3.586958 |
| S | -4.041130 | 0.006282 | 4.508360 |
| S | 0.718230 | 0.763700 | 4.816727 |
| S | 4.374576 | 3.097353 | 2.547757 |
| S | 4.094944 | 2.775010 | -1.272002 |
| S | -4.173073 | 2.403163 | 1.585944 |
| C | -3.367547 | 2.225897 | -4.711977 |
| C | -0.677693 | -6.340802 | -1.995036 |
| C | 0.393376 | 3.347481 | -5.475506 |
| C | 4.546092 | 0.509919 | -6.363936 |
| C | -0.944692 | -2.479557 | -6.066831 |
| C | -4.861209 | -3.252335 | -5.107404 |
| C | -4.605981 | -3.879813 | 0.539724 |
| C | 4.363665 | -3.456173 | -2.924305 |
| C | 3.507518 | -1.910771 | 4.325705 |
| C | 0.371152 | 6.427017 | 1.110852 |
| C | 2.737356 | -6.657023 | 2.066053 |
| C | -0.264749 | -3.293187 | 5.041096 |
| C | -4.331503 | -1.495284 | 5.689571 |
| C | 0.668465 | 2.550037 | 5.554308 |
| C | 4.736871 | 3.364552 | 4.429594 |
| C | 5.868925 | 2.322333 | -0.639143 |
| C | -4.015676 | 3.430860 | 3.223122 |
| C | -4.927693 | 6.408129 | -1.945403 |
| C | -6.034044 | 6.605489 | -3.004073 |
| C | -4.821682 | 4.726628 | 3.133361 |
| C | -4.772855 | 5.503481 | 4.466206 |
| C | -6.342795 | -3.448261 | -5.439536 |
| C | -7.200623 | -2.183058 | -5.265459 |
| C | -5.817706 | -1.852202 | 5.732617 |
| C | -5.576769 | -4.372424 | 1.612107 |
| C | -6.076240 | -3.048989 | 6.673712 |
| C | -5.443292 | -5.895505 | 1.827973 |
| C | -0.956942 | -2.743505 | 6.286185 |
| C | 3.235774 | -5.636909 | 3.083268 |
| C | 0.049249 | -2.552638 | 7.441575 |

| | | | |
|---|---|---|---|
| C | 4.173910 | -6.293005 | 4.119229 |
| C | -0.176753 | -2.590050 | -7.383552 |
| C | 5.339350 | -4.550052 | -2.488744 |
| C | -0.267454 | -4.015907 | -7.968701 |
| C | 5.784168 | -5.414975 | -3.687699 |
| C | -0.037452 | 2.573403 | 6.909348 |
| C | 4.665732 | 4.850498 | 4.784136 |
| C | -0.020672 | 3.987641 | 7.527750 |
| C | 5.060680 | 5.101877 | 6.255275 |
| C | 1.262820 | 7.310041 | 1.983743 |
| C | 1.565261 | 8.654052 | 1.285643 |
| C | 6.121115 | 0.835234 | -0.423532 |
| C | 7.562254 | 0.575899 | 0.064849 |
| C | 3.799760 | 1.811616 | -6.627068 |
| C | 0.418631 | 4.648003 | -6.279135 |
| C | -4.375594 | 1.781827 | -5.772538 |
| C | -0.209587 | 4.455982 | -7.676479 |
| C | -5.726776 | 2.514487 | -5.721069 |
| C | 4.713889 | -1.399297 | 5.117559 |
| C | 6.033478 | -2.135318 | 4.828327 |
| C | -1.767029 | -6.421741 | -0.928870 |
| C | -2.055863 | -7.887301 | -0.538033 |
| H | 2.162703 | -7.461678 | 2.547082 |
| H | 2.364871 | -5.187401 | 3.590051 |
| H | 3.761271 | -4.825246 | 2.554086 |
| H | 3.662050 | -7.103651 | 4.662760 |
| H | 5.066635 | -6.717250 | 3.632536 |
| H | 4.515111 | -5.554315 | 4.860007 |
| H | 0.177624 | -4.280699 | 5.231868 |
| H | 0.505724 | -2.605825 | 4.674867 |
| H | -1.762600 | -3.427832 | 6.600986 |
| H | -1.412312 | -1.767104 | 6.040896 |
| H | 0.531844 | -3.506292 | 7.711892 |
| H | 0.832836 | -1.832533 | 7.159322 |
| H | -0.460465 | -2.164390 | 8.337229 |
| H | -5.262820 | 5.680137 | -1.187884 |
| H | -4.735475 | 7.361122 | -1.424717 |
| H | -6.960359 | 6.964216 | -2.529383 |
| H | -6.262089 | 5.657949 | -3.516578 |
| H | -5.732120 | 7.345705 | -3.762463 |
| C | -3.635004 | 5.900963 | -2.585088 |
| H | -3.772641 | 4.909077 | -3.030071 |
| H | -3.244535 | 6.601842 | -3.337089 |
| H | -2.949288 | 3.624753 | 3.390143 |
| H | -4.400891 | 2.764289 | 4.005926 |
| H | -4.412876 | 5.350993 | 2.321172 |

| | | | |
|---|---|---|---|
| H | -5.199104 | 4.906734 | 5.288313 |
| H | -5.350003 | 6.438148 | 4.389649 |
| H | -3.736060 | 5.763654 | 4.731334 |
| H | -5.868837 | 4.496632 | 2.874463 |
| H | 1.010970 | 4.335501 | 7.696264 |
| H | -0.521424 | 4.712575 | 6.867159 |
| H | -0.542814 | 3.992474 | 8.497091 |
| H | 0.449392 | 1.859745 | 7.594788 |
| H | -1.079457 | 2.236583 | 6.776652 |
| H | 1.724236 | 2.842821 | 5.641431 |
| H | 0.177988 | 3.200849 | 4.821518 |
| H | -6.162043 | -2.098971 | 4.714669 |
| H | -3.960274 | -1.173004 | 6.672495 |
| H | -5.763518 | -2.818945 | 7.705051 |
| H | -3.723939 | -2.326747 | 5.313688 |
| H | -6.400802 | -0.979249 | 6.070201 |
| H | -5.524460 | -3.941467 | 6.338742 |
| H | -7.148164 | -3.299112 | 6.692787 |
| H | 2.597765 | -1.367400 | 4.605261 |
| H | 6.333307 | -2.014183 | 3.776748 |
| H | 5.937195 | -3.213471 | 5.034319 |
| H | 6.844301 | -1.741144 | 5.460831 |
| H | 4.835895 | -0.319452 | 4.922133 |
| H | 4.459796 | -1.504412 | 6.189745 |
| H | 3.359603 | -2.991300 | 4.460263 |
| H | 4.920907 | -5.913183 | -4.156424 |
| H | 6.490671 | -6.193500 | -3.359980 |
| H | 6.284565 | -4.802786 | -4.454803 |
| H | 6.221929 | -4.090331 | -2.013541 |
| H | 4.855624 | -5.187408 | -1.728920 |
| H | 4.816230 | -2.768969 | -3.649128 |
| H | 3.434693 | -3.868489 | -3.336681 |
| C | 4.382324 | 2.558013 | -7.846111 |
| H | 3.853627 | 2.450260 | -5.729624 |
| H | 2.737120 | 1.578218 | -6.802368 |
| H | 5.611643 | 0.686457 | -6.157824 |
| H | 4.449384 | -0.192910 | -7.204087 |
| H | 3.833487 | 3.494987 | -8.024732 |
| H | 5.441516 | 2.813829 | -7.683589 |
| H | 4.313894 | 1.944206 | -8.758625 |
| H | 0.959863 | 2.547486 | -5.970168 |
| H | -0.628216 | 2.996591 | -5.297872 |
| H | -0.128524 | 5.430651 | -5.727314 |
| H | 1.459083 | 4.997728 | -6.382944 |
| H | -0.180524 | 5.396651 | -8.248019 |
| H | 0.332916 | 3.690002 | -8.253223 |

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|---|---|---|---|
| H | -1.261295 | 4.138098 | -7.597570 |
| H | -0.572251 | -1.859978 | -8.109368 |
| H | 0.879933 | -2.329040 | -7.202574 |
| H | -1.312662 | -4.293881 | -8.180070 |
| H | 0.298616 | -4.084534 | -8.910640 |
| H | 0.148244 | -4.755941 | -7.266728 |
| H | -0.547601 | -3.159060 | -5.303638 |
| H | -2.016906 | -2.677796 | -6.203988 |
| H | -4.427938 | -2.403802 | -5.650264 |
| H | -4.281043 | -4.162051 | -5.307124 |
| H | -6.393927 | -3.786704 | -6.491968 |
| H | -6.750469 | -4.268153 | -4.823614 |
| H | -8.242506 | -2.377745 | -5.564412 |
| H | -7.205580 | -1.845751 | -4.218571 |
| H | -6.815699 | -1.359865 | -5.888013 |
| H | -1.450297 | -5.856457 | -0.035059 |
| H | -2.850763 | -7.936040 | 0.222005 |
| H | -2.382282 | -8.476118 | -1.410970 |
| H | -2.684210 | -5.942060 | -1.311532 |
| H | 0.256315 | -6.806352 | -1.652329 |
| H | -1.155838 | -8.364281 | -0.118077 |
| H | -1.000319 | -6.813933 | -2.934721 |
| H | -4.424205 | -6.156521 | 2.153225 |
| H | -6.146181 | -6.238901 | 2.603314 |
| H | -5.664043 | -6.448303 | 0.900993 |
| H | -3.561222 | -4.045265 | 0.825239 |
| H | -4.800403 | -4.348902 | -0.434608 |
| H | -6.611046 | -4.124187 | 1.320500 |
| H | -5.366923 | -3.844076 | 2.556864 |
| H | 4.017243 | 2.768039 | 5.002396 |
| H | 5.747942 | 2.957913 | 4.577793 |
| H | 3.641978 | 5.217113 | 4.600999 |
| H | 4.994664 | 6.174737 | 6.494034 |
| H | 6.094426 | 4.773872 | 6.450030 |
| H | 4.394560 | 4.559419 | 6.944526 |
| H | 6.531755 | 2.738124 | -1.413100 |
| H | 5.404020 | 0.448758 | 0.322904 |
| H | 5.932837 | 0.286307 | -1.361679 |
| H | 7.725040 | -0.501984 | 0.218157 |
| H | 8.303116 | 0.933070 | -0.669396 |
| H | 5.986721 | 2.895296 | 0.290008 |
| H | 7.752601 | 1.088742 | 1.021445 |
| H | -3.193824 | 3.311404 | -4.741134 |
| H | -2.420013 | 1.689783 | -4.826855 |
| H | -3.900194 | 1.949358 | -6.757636 |
| H | -4.531814 | 0.693703 | -5.675031 |

| | | | |
|---|---|---|---|
| H | -5.587549 | 3.603036 | -5.823146 |
| H | -6.246858 | 2.321138 | -4.771137 |
| H | -6.381457 | 2.179745 | -6.540689 |
| H | 0.858701 | 6.161882 | 0.165181 |
| H | -0.593474 | 6.908605 | 0.900012 |
| H | 2.205591 | 6.776825 | 2.193229 |
| H | 0.768697 | 7.494504 | 2.952721 |
| H | 2.079749 | 8.491132 | 0.325446 |
| H | 2.212828 | 9.282352 | 1.917147 |
| H | 0.637693 | 9.213920 | 1.085589 |
| H | 5.336903 | 5.419447 | 4.119228 |
| H | 3.566117 | -7.095243 | 1.491855 |

**$[Au_{25}(SR)_{18}]^{1-}$ $S_0$**

| | | | |
|---|---|---|---|
| Au | -0.001750 | 0.000369 | 0.000873 |
| Au | -1.956746 | 1.594127 | -1.339858 |
| Au | -2.501313 | -1.294245 | -0.287945 |
| Au | 0.133856 | -2.777692 | -0.453851 |
| Au | -0.876677 | -0.854626 | -2.539268 |
| Au | -4.124330 | -0.618068 | -2.666525 |
| Au | 2.111891 | -0.947917 | -1.634859 |
| Au | 1.441709 | -0.249151 | -4.560292 |
| Au | -2.207419 | -3.563853 | -2.390662 |
| Au | 0.910446 | 1.546642 | -2.172735 |
| Au | -4.010829 | -1.181852 | 2.568898 |
| Au | -3.072519 | 3.769949 | 0.378956 |
| Au | -0.581623 | 4.259546 | -2.137824 |
| Au | 1.953263 | -1.593096 | 1.341389 |
| Au | 2.498353 | 1.295345 | 0.287352 |
| Au | -0.137786 | 2.779121 | 0.454221 |
| Au | 0.873913 | 0.855264 | 2.539855 |
| Au | 4.121491 | 0.619286 | 2.664840 |
| Au | -2.115750 | 0.949049 | 1.635872 |
| Au | -1.443549 | 0.250354 | 4.559317 |
| Au | 2.206369 | 3.564050 | 2.390205 |
| Au | -0.913688 | -1.545462 | 2.174936 |
| Au | 4.006830 | 1.180700 | -2.572278 |
| Au | 3.065346 | -3.767766 | -0.377205 |
| Au | 0.573686 | -4.258784 | 2.136492 |
| S | -4.091049 | 1.805953 | -2.692534 |
| S | -0.068566 | -4.685161 | -2.128095 |
| S | -2.292470 | 5.587261 | -1.026134 |
| S | 1.245883 | 3.600394 | -3.627154 |
| S | 3.836342 | 0.126091 | -4.755121 |
| S | -0.885771 | -0.788318 | -5.070425 |
| S | -4.534855 | -3.008971 | -2.813144 |

| | | | |
|---|---|---|---|
| S | -4.665591 | -2.333457 | 0.550703 |
| S | 4.211245 | -2.335626 | -1.954544 |
| S | 4.089498 | -1.804978 | 2.689436 |
| S | 0.065411 | 4.683066 | 2.131304 |
| S | 2.286421 | -5.586598 | 1.027274 |
| S | -1.251448 | -3.599527 | 3.628814 |
| S | -3.837528 | -0.131641 | 4.753924 |
| S | 0.882332 | 0.795761 | 5.071252 |
| S | 4.534370 | 3.009739 | 2.810193 |
| S | 4.661035 | 2.334414 | -0.554830 |
| S | -4.214279 | 2.338328 | 1.959103 |
| C | -3.556681 | 2.075884 | -4.529981 |
| C | -0.567796 | -6.298274 | -1.185245 |
| C | -3.700358 | 5.683560 | -2.347020 |
| C | 0.310991 | 3.195776 | -5.269293 |
| C | 3.975458 | 1.649477 | -5.935363 |
| C | -0.711454 | -2.612502 | -5.684113 |
| C | -4.744508 | -3.409455 | -4.694279 |
| C | -4.087894 | -4.142485 | 0.913204 |
| C | 3.992603 | -3.381493 | -3.567059 |
| C | 3.556115 | -2.076784 | 4.527010 |
| C | 0.560933 | 6.299324 | 1.192520 |
| C | 3.694111 | -5.677212 | 2.349063 |
| C | -0.311277 | -3.197209 | 5.268700 |
| C | -3.968663 | -1.657913 | 5.931394 |
| C | 0.703301 | 2.622274 | 5.676946 |
| C | 4.746699 | 3.414188 | 4.689937 |
| C | 4.080739 | 4.143051 | -0.915787 |
| C | -3.991369 | 3.383375 | 3.571688 |
| C | -4.680727 | 1.664976 | -5.484249 |
| C | -4.296133 | 1.895357 | -6.961385 |
| C | 4.682432 | -1.671340 | 5.480798 |
| C | 4.298369 | -1.903180 | 6.957812 |
| C | -1.154748 | -7.339554 | -2.138364 |
| H | -2.073290 | -6.937134 | -2.597591 |
| C | 1.137168 | 7.342432 | 2.150132 |
| H | 2.054400 | 6.943833 | 2.615285 |
| C | -4.994024 | 6.212291 | -1.725302 |
| C | -6.110950 | 6.341606 | -2.784755 |
| C | 4.990083 | -6.201448 | 1.728263 |
| C | 6.108153 | -6.322064 | 2.787570 |
| C | 0.114681 | 4.456558 | -6.113316 |
| H | -0.488415 | 5.183468 | -5.543583 |
| C | -0.121938 | -4.457768 | 6.114512 |
| H | 0.475863 | -5.189560 | 5.545491 |
| C | 5.433856 | 2.097963 | -6.047838 |

| | | | |
|---|---|---|---|
| C | 5.576608 | 3.329941 | -6.967722 |
| C | -5.425027 | -2.111591 | 6.049591 |
| C | -5.558300 | -3.345363 | 6.968664 |
| C | -0.005493 | -2.683108 | -7.038414 |
| C | 0.082810 | -4.136884 | -7.551936 |
| C | -0.008606 | 2.698775 | 7.027763 |
| C | -0.099785 | 4.155146 | 7.533411 |
| C | -6.212702 | -3.279029 | -5.105265 |
| C | -6.422430 | -3.684512 | -6.580358 |
| C | 6.211310 | 3.260672 | 5.106102 |
| C | 6.425144 | 3.677370 | 6.577543 |
| C | -4.902011 | -4.781918 | 2.038662 |
| C | -4.468971 | -6.244223 | 2.283863 |
| C | 4.897738 | 4.787141 | -2.036371 |
| C | 4.463007 | 6.249592 | -2.277503 |
| C | 4.856611 | -4.643013 | -3.515134 |
| C | 4.760149 | -5.449915 | -4.827864 |
| C | -4.858105 | 4.643350 | 3.524988 |
| C | -4.760068 | 5.448263 | 4.838857 |
| H | -2.652646 | 1.481346 | -4.705834 |
| H | -3.321519 | 3.147142 | -4.615142 |
| H | -5.599519 | 2.225624 | -5.242119 |
| H | -4.902457 | 0.596653 | -5.320860 |
| H | 3.317938 | -3.147511 | 4.610427 |
| H | 2.653937 | -1.480040 | 4.704919 |
| H | 5.599068 | -2.234745 | 5.236875 |
| H | 4.907755 | -0.603495 | 5.319246 |
| H | -1.272829 | -6.021919 | -0.392722 |
| H | 0.365433 | -6.653922 | -0.728157 |
| C | -1.469142 | -8.659502 | -1.399679 |
| H | -0.439330 | -7.532926 | -2.955643 |
| H | -0.371460 | 6.650574 | 0.730463 |
| H | 1.271932 | 6.027396 | 0.403823 |
| C | 1.451036 | 8.663855 | 1.413951 |
| H | 0.415520 | 7.532417 | 2.962710 |
| H | -3.839775 | 4.671251 | -2.743940 |
| H | -3.318152 | 6.351071 | -3.133359 |
| H | -4.808491 | 7.192958 | -1.255015 |
| H | -5.314483 | 5.519555 | -0.929469 |
| H | 3.313903 | -6.345205 | 3.135978 |
| H | 3.829859 | -4.663899 | 2.744767 |
| H | 4.809244 | -7.184305 | 1.260738 |
| H | 5.306872 | -5.509298 | 0.930430 |
| H | -0.643297 | 2.728395 | -5.004008 |
| H | 0.931846 | 2.446938 | -5.783214 |
| C | -0.579131 | 4.136345 | -7.455579 |

| | | | |
|---|---|---|---|
| H | 1.092965 | 4.929637 | -6.304363 |
| H | -0.926309 | -2.443378 | 5.782318 |
| H | 0.645559 | -2.736555 | 5.000846 |
| C | 0.575574 | -4.138735 | 7.455038 |
| H | -1.102862 | -4.924319 | 6.307972 |
| H | 3.344717 | 2.444416 | -5.518555 |
| H | 3.572664 | 1.318105 | -6.903452 |
| H | 5.813371 | 2.339120 | -5.041092 |
| H | 6.047671 | 1.267507 | -6.435840 |
| H | -3.563069 | -1.327415 | 6.898555 |
| H | -3.337296 | -2.450108 | 5.510224 |
| H | -5.808394 | -2.352883 | 5.044352 |
| H | -6.040041 | -1.283972 | 6.441736 |
| H | -1.741672 | -2.991487 | -5.742397 |
| H | -0.173576 | -3.175577 | -4.913249 |
| H | -0.544491 | -2.058977 | -7.771369 |
| H | 1.008263 | -2.260727 | -6.935497 |
| H | 0.168390 | 3.181592 | 4.901308 |
| H | 1.732881 | 3.002639 | 5.738057 |
| H | 0.527425 | 2.078491 | 7.766139 |
| H | -1.021751 | 2.275537 | 6.922380 |
| H | -4.381450 | -4.439831 | -4.816357 |
| H | -4.101679 | -2.723589 | -5.258411 |
| H | -6.832615 | -3.918080 | -4.454064 |
| H | -6.545892 | -2.239783 | -4.949579 |
| H | 4.090447 | 2.742630 | 5.255810 |
| H | 4.401076 | 4.451348 | 4.805706 |
| H | 6.844670 | 3.881357 | 4.450096 |
| H | 6.525350 | 2.213839 | 4.961747 |
| H | -3.019862 | -4.107733 | 1.156996 |
| H | -4.228157 | -4.668165 | -0.042709 |
| H | -5.975964 | -4.742386 | 1.788352 |
| H | -4.756962 | -4.193810 | 2.959914 |
| H | 4.216399 | 4.666920 | 0.041848 |
| H | 3.013714 | 4.106670 | -1.163543 |
| H | 5.970876 | 4.748567 | -1.782439 |
| H | 4.756858 | 4.202013 | -2.960182 |
| H | 4.301456 | -2.710735 | -4.380479 |
| H | 2.927660 | -3.622148 | -3.671448 |
| H | 4.529118 | -5.267341 | -2.666838 |
| H | 5.906860 | -4.362422 | -3.326432 |
| H | -2.926478 | 3.625940 | 3.672145 |
| H | -4.295753 | 2.711081 | 4.385517 |
| H | -4.534419 | 5.269906 | 2.676885 |
| H | -5.908275 | 4.360927 | 3.338689 |
| H | 1.863169 | 9.412045 | 2.110074 |

| | | | |
|---|---|---|---|
| H | 2.187930 | 8.500333 | 0.611525 |
| H | 0.540969 | 9.085500 | 0.957243 |
| H | -5.384587 | 6.354897 | 4.787435 |
| H | -5.101319 | 4.846589 | 5.696923 |
| H | -3.720883 | 5.759713 | 5.030503 |
| H | -6.610814 | -3.661992 | 7.041971 |
| H | -4.974557 | -4.192598 | 6.574865 |
| H | -5.197014 | -3.123846 | 7.986528 |
| H | 0.712315 | -5.054886 | 8.051930 |
| H | 1.566399 | -3.689840 | 7.285271 |
| H | -0.019207 | -3.427217 | 8.050550 |
| H | 6.320577 | -5.341889 | 3.243399 |
| H | 7.038704 | -6.690522 | 2.327388 |
| H | 5.823260 | -7.022530 | 3.590000 |
| H | 5.113063 | -1.577889 | 7.625514 |
| H | 3.393165 | -1.333211 | 7.219517 |
| H | 4.105453 | -2.969856 | 7.156136 |
| H | 5.820680 | 3.054864 | 7.256643 |
| H | 6.137857 | 4.730179 | 6.733519 |
| H | 7.482990 | 3.567054 | 6.864574 |
| H | 3.401339 | 6.296340 | -2.567110 |
| H | 5.057902 | 6.705251 | -3.085903 |
| H | 4.601393 | 6.858217 | -1.368860 |
| H | -1.567031 | 3.680068 | -7.288218 |
| H | -0.721618 | 5.053186 | -8.050029 |
| H | 0.021213 | 3.430671 | -8.052475 |
| H | -5.109254 | 1.566255 | -7.629119 |
| H | -4.106384 | 2.962285 | -7.161542 |
| H | -3.388976 | 1.327693 | -7.221322 |
| H | -5.831384 | -3.043813 | -7.254281 |
| H | -7.482875 | -3.591018 | -6.863652 |
| H | -6.115858 | -4.730084 | -6.747882 |
| H | -4.611735 | -6.856297 | 1.378215 |
| H | -3.406395 | -6.291707 | 2.569960 |
| H | -5.061600 | -6.695554 | 3.096370 |
| H | -0.622669 | 4.199461 | 8.502128 |
| H | -0.652678 | 4.783542 | 6.817452 |
| H | 0.903202 | 4.592866 | 7.665453 |
| H | -7.040107 | 6.712591 | -2.323824 |
| H | -6.327497 | 5.364019 | -3.244232 |
| H | -5.822493 | 7.043702 | -3.584533 |
| H | -2.199522 | -8.492749 | -0.592017 |
| H | -1.889496 | -9.406062 | -2.092615 |
| H | -0.557685 | -9.085088 | -0.949434 |
| H | 3.720860 | -5.760003 | -5.021169 |
| H | 5.383072 | -6.357467 | -4.773502 |

| | | | |
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| H | 5.104190 | -4.850240 | -5.686208 |
| H | 5.220285 | 3.108491 | -7.987318 |
| H | 6.630670 | 3.642635 | -7.035454 |
| H | 4.993753 | 4.179774 | -6.578259 |
| H | -0.920958 | -4.573532 | -7.681443 |
| H | 0.638849 | -4.769233 | -6.841921 |
| H | 0.601008 | -4.176437 | -8.523368 |