

Ligand-Core Interaction in Ligand-Protected $\text{Ag}_{25}(\text{XR})_{18}$ (X= S, Se, Te) Superatoms. Evaluation of Anchor Atom Role via Relativistic DFT Calculations

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Table S1. Selected geometrical parameters for $[\text{Ag}_{25}(\text{XMe})_{18}]^-$ (X=S, Se and Te), values in Å. In addition, CShM values and Hirshfeld charge analysis (a.u.) are given.

| | S | Se | Te |
|--------------------------------------|-------|-------|--------|
| CShM | 0.03 | 0.08 | 0.02 |
| Ag-X | 2.439 | 2.581 | 2.670 |
| ^a ∅ Ag ₁₃ | 2.802 | 2.809 | 2.809 |
| ∅ Ag ₁₂ | 4.783 | 4.773 | 4.669 |
| ∅ (XMe) ₁₂ | 5.104 | 5.378 | 5.530 |
| ∅ (XMe) ₆ | 6.221 | 6.353 | 6.610 |
| Hirshfeld | | | |
| Ag ₁₃ | +3.29 | +3.19 | + 3.20 |
| Ag ₁₂ (XMe) ₁₈ | -4.29 | -4.19 | -4.20 |

^aRadius.

Table S2. Selected geometrical parameters for $[\text{Au}_{25}(\text{XMe})_{18}]^-$ ($\text{X}=\text{S}$, Se and Te), values in Å. In addition, CShM values and Hirshfeld charge analysis (a.u.) are given.

| | S | Se | Te |
|--------------------------------------|-------|-------|-------|
| CShM | 0.12 | 0.10 | 0.09 |
| Au-X | 2.453 | 2.562 | 2.672 |
| Au13-Au | 3.392 | 3.393 | 3.562 |
| ^a Ø Au ₁₃ | 2.851 | 2.833 | 2.822 |
| Ø Au ₁₂ | 5.085 | 5.164 | 5.362 |
| Ø (SMe) ₁₂ | 5.155 | 5.305 | 5.463 |
| Ø (SMe) ₆ | 6.266 | 6.401 | 6.792 |
| Hirshfeld | | | |
| Au ₁₃ | +2.65 | +2.54 | +1.95 |
| Au ₁₂ (SMe) ₁₈ | -3.65 | -3.54 | -3.95 |

^aRadius.

Note: $[\text{Au}_{25}(\text{XMe})_{18}]^-$ ($\text{X}=\text{S}$, Se and Te), results taken from reference A. Muñoz-Castro, *Phys. Chem. Chem. Phys.*, 2019, **21**, 13022–13029.

Table S3. Energy decomposition analysis for the interaction involving the overall interaction between $[\text{Au}_{13}]^{5+}$ and the protecting layer (PL^{6-}), at the ground state (S_0). Further decomposition of the ΔE_{orb} term is evaluated via EDA-NOCV calculations. Values in $\text{kcal}\cdot\text{mol}^{-1}$. In addition, the percentual contribution to the overall orbital term is given.

| S_0 | S | | Se | | Te | |
|----------------------------|---------|-------|---------|-------|---------|-------|
| ΔE_{Pauli} | 1392.4 | | 1320.6 | | 1185.3 | |
| ΔE_{elstat} | -2639.5 | 67.5% | -2568.4 | 67.0% | -2500.2 | 66.6% |
| ΔE_{orb} | -1086.9 | 27.8% | -1053.2 | 27.5% | -1024.3 | 27.3% |
| ΔE_{disp} | -185.1 | 4.7% | -212.6 | 5.5% | -229.0 | 6.1% |
| ΔE_{int} | -2519.1 | | -2513.5 | | -2568.2 | |
| ΔE_{orb} | | | | | | |
| $\Delta\rho_1$ | -62.2 | 5.7% | -67.9 | 6.4% | -71.5 | 7.0% |
| $\Delta\rho_2$ | -61.8 | 5.7% | -67.4 | 6.4% | -72.0 | 7.0% |
| $\Delta\rho_3$ | -61.3 | 5.6% | -66.8 | 6.3% | -71.2 | 7.0% |
| $\Delta\rho_4$ | -62.8 | 5.8% | -65.5 | 6.2% | -70.6 | 6.9% |
| $\Delta\rho_5$ | -60.6 | 5.6% | -65.9 | 6.3% | -69.2 | 6.8% |
| $\Delta\rho_6$ | -43.6 | 4.0% | -44.5 | 4.2% | -47.3 | 4.6% |
| $\Delta\rho_7$ | -43.7 | 4.0% | -44.9 | 4.3% | -47.3 | 4.6% |
| $\Delta\rho_8$ | -43.8 | 4.0% | -44.7 | 4.2% | -47.5 | 4.6% |
| $\Delta\rho_9$ | -44.8 | 4.1% | -49.7 | 4.7% | -54.2 | 5.3% |
| | | | | | | |

Table S4. Selected geometrical parameters for $[\text{Ag}_{25}(\text{XMe})_{18}]^-$ (X=S, Se and Te), values in Å, as calculated at the non-relativistic level of theory. In addition, CShM values and Hirshfeld charge analysis (a.u.) are given.

| | S | Se | Te |
|--------------------------------------|-------|-------|--------|
| CShM | 0.03 | 0.06 | 0.03 |
| Ag-X | 2.606 | 2.682 | 2.67 |
| ^a Ø Ag ₁₃ | 2.837 | 2.849 | 2.861 |
| Ø Ag ₁₂ | 4.858 | 4.845 | 4.879 |
| Ø (XMe) ₁₂ | 5.329 | 5.453 | 5.683 |
| Ø (XMe) ₆ | 6.375 | 6.680 | 7.020 |
| Hirshfeld | | | |
| Ag ₁₃ | +3.67 | +3.59 | + 3.43 |
| Ag ₁₂ (XMe) ₁₈ | -4.67 | -4.59 | -4.43 |

^aRadius.

Table S5. Selected geometrical parameters for the S₁ excited state for $[\text{Ag}_{25}(\text{XMe})_{18}]^-$ (X=S, Se and Te), values in Å, as calculated. In addition, CShM values and Hirshfeld charge analysis (a.u.) are given.

| | S | Se | Te |
|--------------------------------------|-------|-------|--------|
| CShM | 0.13 | 0.09 | 0.02 |
| Ag-X | 2.481 | 2.608 | 2.759 |
| ^a Ø Ag ₁₃ | 2.845 | 2.801 | 2.812 |
| Ø Ag ₁₂ | 5.075 | 4.776 | 4.640 |
| Ø (XMe) ₁₂ | 5.110 | 5.358 | 5.538 |
| Ø (XMe) ₆ | 6.301 | 6.498 | 6.691 |
| Hirshfeld | | | |
| Ag ₁₃ | +3.34 | +3.19 | + 3.21 |
| Ag ₁₂ (XMe) ₁₈ | -4.34 | -4.19 | -4.21 |

^aRadius.

Table S6. Energy decomposition analysis for the interaction involving the overall interaction between $[\text{Ag}_{13}]^{5+}$ and the protecting layer (PL^{6-}), at the first singlet excited state (S_1). Further decomposition of the ΔE_{orb} term is evaluated via EDA-NOCV calculations. Values in $\text{kcal}\cdot\text{mol}^{-1}$. In addition, the percentual contribution to the overall orbital term is given.

| S_1 | S | | Se | | Te | |
|----------------------------|---------|-------|---------|-------|---------|-------|
| ΔE_{Pauli} | 1161.7 | | 1225.4 | | 1283.5 | |
| ΔE_{elstat} | -2459.4 | 72.2% | -2455.8 | 70.8% | -2404.6 | 68.7% |
| ΔE_{orb} | -855.5 | 25.1% | -914.6 | 26.4% | -996.9 | 28.5% |
| ΔE_{disp} | -92.6 | 2.7% | -96.2 | 2.8% | -99.9 | 2.9% |
| ΔE_{int} | -2245.8 | | -2241.1 | | -2217.8 | |
| ΔE_{orb} | | | | | | |
| $\Delta\rho_1$ | -73.5 | 8.6% | -33.7 | 3.7% | -40.5 | 4.1% |
| $\Delta\rho_2$ | -62.1 | 7.3% | -29.3 | 3.2% | -33.6 | 3.4% |
| $\Delta\rho_3$ | -42.9 | 5.0% | -24.9 | 2.7% | -29.6 | 3.0% |
| $\Delta\rho_4$ | -42.9 | 5.0% | -24.5 | 2.7% | -28.1 | 2.8% |
| $\Delta\rho_5$ | -42.6 | 5.0% | -23.8 | 2.6% | -28.0 | 2.8% |
| $\Delta\rho_6$ | -42.4 | 5.0% | -15.2 | 1.7% | -17.7 | 1.8% |
| $\Delta\rho_7$ | -36.8 | 4.3% | -14.0 | 1.5% | -17.2 | 1.7% |
| $\Delta\rho_8$ | -26.4 | 3.1% | -12.8 | 1.4% | -13.8 | 1.4% |
| $\Delta\rho_9$ | -26.0 | 3.0% | -11.5 | 1.3% | -12.6 | 1.3% |
| | | | | | | |

Table S7. Energy decomposition analysis for the interaction involving the overall interaction between $[\text{Au}_{13}]^{5+}$ and the protecting layer (PL^{6-}), at the first singlet excited state (S_1). Further decomposition of the ΔE_{orb} term is evaluated via EDA-NOCV calculations. Values in $\text{kcal}\cdot\text{mol}^{-1}$. In addition, the percentual contribution to the overall orbital term is given.

| S_1 | S | | Se | | Te | |
|----------------------------|---------|-------|---------|-------|---------|-------|
| ΔE_{Pauli} | 1458.3 | | 1390.2 | | 1375.7 | |
| ΔE_{Elstat} | -2714.4 | 68.0% | -2555.1 | 69.5% | -2557.8 | 65.4% |
| ΔE_{Orb} | -1096.1 | 27.4% | -910.9 | 24.8% | -1136.4 | 29.0% |
| ΔE_{Disp} | -183.1 | 4.6% | -208.6 | 5.7% | -218.0 | 5.6% |
| ΔE_{int} | -2535.3 | | -2284.3 | | -2536.6 | |
| ΔE_{Orb} | | | | | | |
| $\Delta\rho_1$ | -62.2 | 5.7% | -67.9 | 7.5% | -71.5 | 6.3% |
| $\Delta\rho_2$ | -61.8 | 5.6% | -67.4 | 7.4% | -72.0 | 6.3% |
| $\Delta\rho_3$ | -61.3 | 5.6% | -66.8 | 7.3% | -71.2 | 6.3% |
| $\Delta\rho_4$ | -62.8 | 5.7% | -65.5 | 7.2% | -70.6 | 6.2% |
| $\Delta\rho_5$ | -60.6 | 5.5% | -65.9 | 7.2% | -69.2 | 6.1% |
| $\Delta\rho_6$ | -43.6 | 4.0% | -44.5 | 4.9% | -47.3 | 4.2% |
| $\Delta\rho_7$ | -43.7 | 4.0% | -44.9 | 4.9% | -47.3 | 4.2% |
| $\Delta\rho_8$ | -43.8 | 4.0% | -44.7 | 4.9% | -47.5 | 4.2% |
| $\Delta\rho_9$ | -44.8 | 4.1% | -49.7 | 5.5% | -54.2 | 4.8% |
| | | | | | | |

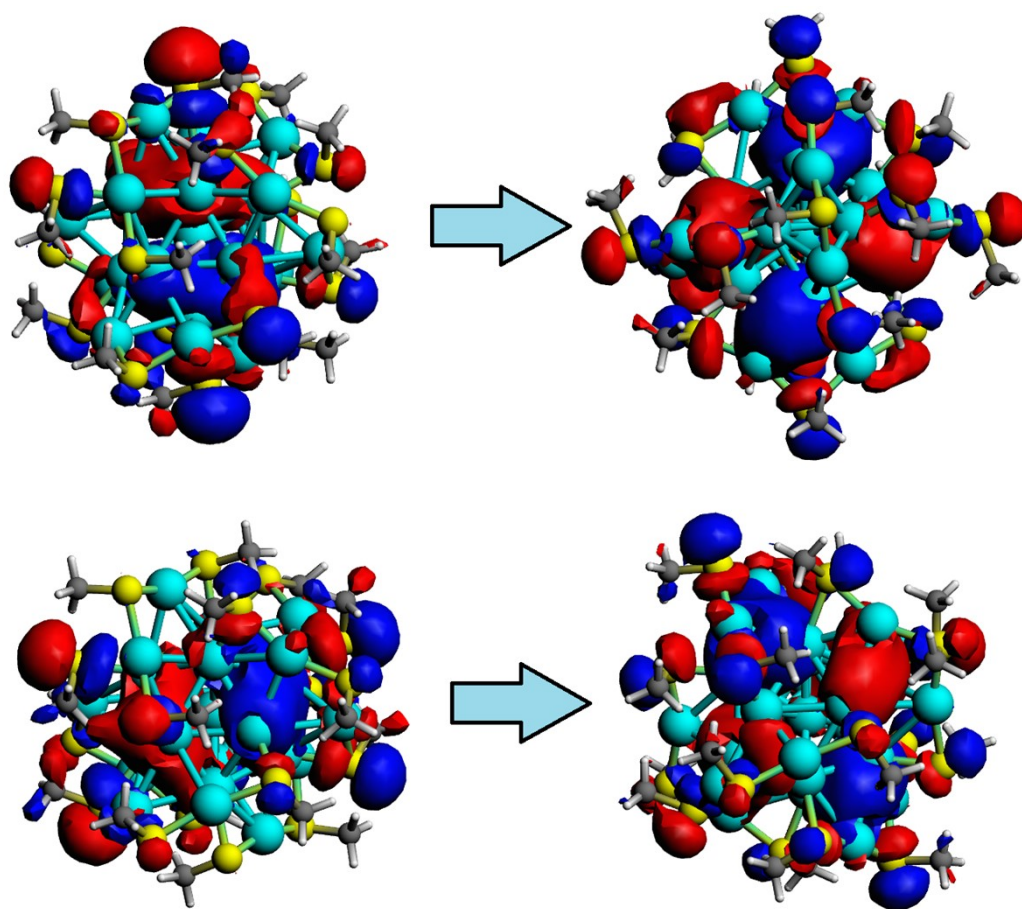


Figure S1. Natural transition orbitals related to the first excitation depicted on the calculated optical absorption spectrum for [Ag₂₅(SMe)₁₈]⁻.

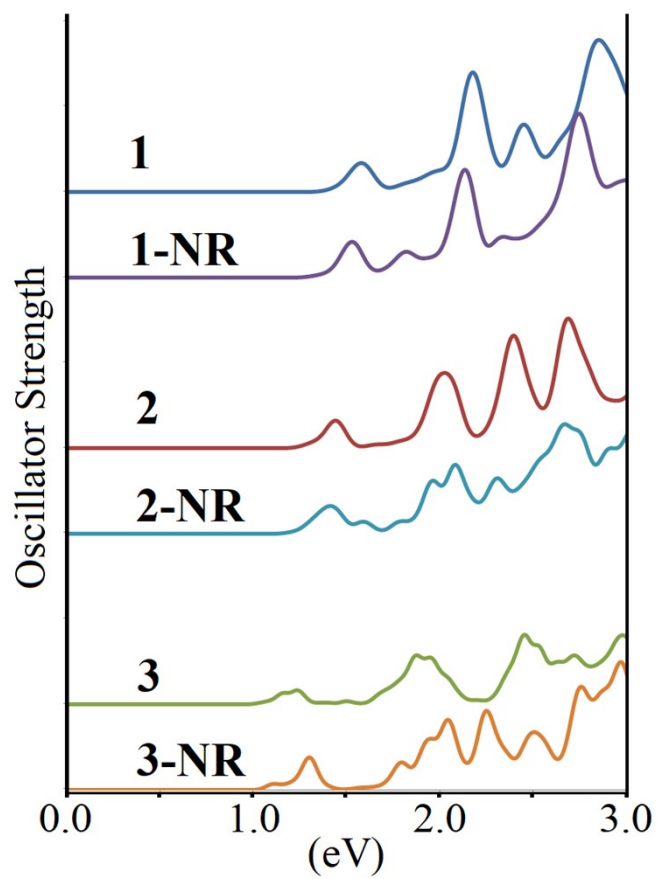


Figure S2. Calculated optical absorption spectrum for $[Ag_{25}(XMe)_{18}]^-$ with $X=S$ (1), Se (2) and Te (3), and the respective results obtained at the non-relativistic case (NR).

Table S8. Coordinates for the calculated species, given in Angstroms (Å).

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Ag₂₅(SMe)₁₈- S₀ Ground State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.051033000 | 0.055484000 | -0.063962000 |
| Ag | -2.059387000 | 1.646413000 | -1.210718000 |
| Ag | -0.780584000 | -2.369675000 | 1.134015000 |
| Ag | 0.711260000 | 2.466399000 | -1.238520000 |
| Ag | 1.977482000 | -1.523703000 | 1.097609000 |
| Ag | -2.142456000 | -1.318025000 | -1.305906000 |
| Ag | 2.453302000 | 0.109518000 | -1.375160000 |
| Ag | -2.563690000 | 0.028859000 | 1.196389000 |
| Ag | 2.050568000 | 1.442238000 | 1.131762000 |
| Ag | -0.123795000 | 0.067877000 | -2.875371000 |
| Ag | -0.743081000 | 2.384394000 | 1.316182000 |
| Ag | 0.642902000 | -2.287193000 | -1.408834000 |
| Ag | -0.014745000 | -0.010275000 | 2.737557000 |
| Ag | 3.640862000 | 2.948712000 | -1.022846000 |
| S | 5.799941000 | 2.029589000 | -0.361235000 |
| Ag | 4.713901000 | 0.150871000 | 0.769446000 |
| C | 6.544995000 | 1.320953000 | -1.892209000 |
| H | 7.461865000 | 0.789359000 | -1.607701000 |
| H | 5.849928000 | 0.620128000 | -2.375037000 |
| H | 6.793840000 | 2.141968000 | -2.576830000 |
| Ag | -4.773838000 | 0.046925000 | -0.934147000 |
| S | -5.897496000 | -1.895592000 | 0.031894000 |
| Ag | -3.772667000 | -2.963866000 | 0.622097000 |
| C | -6.718913000 | -1.353923000 | 1.587658000 |
| H | -7.602322000 | -0.758580000 | 1.327578000 |
| H | -6.034449000 | -0.751146000 | 2.200240000 |
| H | -7.029197000 | -2.247753000 | 2.141410000 |
| Ag | -2.204241000 | 1.676837000 | 3.902431000 |
| S | -0.777936000 | 3.360619000 | 4.938300000 |
| Ag | 1.221075000 | 2.576069000 | 3.757072000 |
| C | -0.406459000 | 2.676250000 | 6.618850000 |
| H | 0.297163000 | 3.354501000 | 7.117007000 |
| H | 0.050002000 | 1.682648000 | 6.534724000 |
| H | -1.335155000 | 2.616554000 | 7.198839000 |
| Ag | -1.301082000 | -2.605061000 | -3.837552000 |
| S | 0.479222000 | -2.992746000 | -5.461338000 |
| Ag | 2.079531000 | -1.939291000 | -3.953461000 |
| C | 0.199499000 | -1.787089000 | -6.829614000 |
| H | 1.060703000 | -1.835320000 | -7.506323000 |
| H | 0.097939000 | -0.767289000 | -6.436018000 |
| H | -0.709234000 | -2.074191000 | -7.372663000 |
| Ag | 1.350538000 | -4.488202000 | 0.638451000 |
| S | 1.413521000 | -4.954382000 | 3.044101000 |
| Ag | 0.899317000 | -2.664144000 | 3.705375000 |
| C | 3.212128000 | -5.068035000 | 3.441144000 |
| H | 3.337641000 | -5.057161000 | 4.530413000 |
| H | 3.757974000 | -4.229094000 | 2.989004000 |
| H | 3.592844000 | -6.013324000 | 3.035872000 |
| Ag | -0.744542000 | 3.083794000 | -3.728822000 |
| S | -1.624027000 | 5.253213000 | -3.073068000 |
| Ag | -1.433761000 | 4.619951000 | -0.715437000 |
| C | -3.416276000 | 5.213855000 | -3.499331000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.907225000 | 6.064988000 | -3.012073000 |
| H | -3.874523000 | 4.276200000 | -3.153848000 |
| H | -3.518697000 | 5.302623000 | -4.587359000 |
| S | -3.299680000 | -3.230057000 | -2.511755000 |
| S | -4.012052000 | 0.170228000 | 3.251567000 |
| S | 4.082884000 | -1.157821000 | -2.801670000 |
| S | 3.538900000 | 2.305543000 | 2.982344000 |
| S | -4.246418000 | 1.921107000 | -2.431865000 |
| S | -2.020149000 | -4.547482000 | 1.293189000 |
| S | 1.926942000 | 4.676673000 | -1.450545000 |
| S | 4.272773000 | -1.901065000 | 2.030132000 |
| S | 1.340176000 | -4.667088000 | -1.815365000 |
| S | 0.700002000 | -0.625590000 | 5.100467000 |
| S | 0.331832000 | 1.312718000 | -5.016597000 |
| S | -1.272640000 | 4.792482000 | 1.733489000 |
| C | -0.856128000 | -0.871080000 | 6.070934000 |
| H | -1.308073000 | -1.843133000 | 5.853286000 |
| H | -0.600911000 | -0.820398000 | 7.137048000 |
| H | -1.576140000 | -0.076584000 | 5.826512000 |
| C | -0.315322000 | -5.458106000 | -2.065583000 |
| H | -1.065190000 | -5.039895000 | -1.385887000 |
| H | -0.225045000 | -6.534272000 | -1.880179000 |
| H | -0.627740000 | -5.284582000 | -3.102368000 |
| C | 0.447231000 | 5.455617000 | 1.882555000 |
| H | 1.106507000 | 5.014083000 | 1.127091000 |
| H | 0.426334000 | 6.542072000 | 1.741962000 |
| H | 0.819286000 | 5.215017000 | 2.886993000 |
| C | 2.137568000 | 1.626367000 | -4.769943000 |
| H | 2.364095000 | 1.823322000 | -3.713095000 |
| H | 2.445317000 | 2.479674000 | -5.384364000 |
| H | 2.687385000 | 0.728895000 | -5.080967000 |
| C | 4.031155000 | 3.979260000 | 2.363202000 |
| H | 3.236999000 | 4.434621000 | 1.763601000 |
| H | 4.258925000 | 4.623732000 | 3.219987000 |
| H | 4.926704000 | 3.856517000 | 1.742395000 |
| C | 4.434839000 | -2.567742000 | -1.655545000 |
| H | 3.548436000 | -2.819818000 | -1.059956000 |
| H | 4.740057000 | -3.442342000 | -2.240507000 |
| H | 5.241604000 | -2.262887000 | -0.977849000 |
| C | -3.521798000 | -1.489985000 | 3.894940000 |
| H | -2.461720000 | -1.680980000 | 3.693208000 |
| H | -3.712515000 | -1.545263000 | 4.971343000 |
| H | -4.118550000 | -2.245894000 | 3.366529000 |
| C | -4.772054000 | -2.508136000 | -3.366217000 |
| H | -4.630317000 | -1.442927000 | -3.571421000 |
| H | -4.941331000 | -3.045678000 | -4.306742000 |
| H | -5.636939000 | -2.633028000 | -2.703541000 |
| C | 4.070303000 | -1.212453000 | 3.735168000 |
| H | 3.425797000 | -0.327983000 | 3.730519000 |
| H | 5.054100000 | -0.935330000 | 4.128488000 |
| H | 3.618581000 | -1.982835000 | 4.372219000 |
| C | -2.199398000 | -4.854727000 | 3.107506000 |
| H | -2.341541000 | -3.917616000 | 3.655252000 |
| H | -3.060618000 | -5.512148000 | 3.275516000 |
| H | -1.281999000 | -5.343158000 | 3.457969000 |
| C | 2.070563000 | 5.141257000 | -3.234122000 |

| | | | |
|---|--------------|-------------|--------------|
| H | 2.151380000 | 4.252448000 | -3.867483000 |
| H | 2.956740000 | 5.772965000 | -3.369260000 |
| H | 1.167838000 | 5.699683000 | -3.508645000 |
| C | -3.721483000 | 1.091066000 | -4.000977000 |
| H | -2.995137000 | 0.290775000 | -3.802461000 |
| H | -4.598186000 | 0.682247000 | -4.516394000 |
| H | -3.240108000 | 1.843184000 | -4.639644000 |

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Ag25(SMe)18- S1 Excited State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.052900000 | 0.064452000 | -0.057283000 |
| Ag | -2.058816000 | 1.656747000 | -1.237604000 |
| Ag | -0.803113000 | -2.346797000 | 1.184543000 |
| Ag | 0.729975000 | 2.459704000 | -1.265878000 |
| Ag | 1.964469000 | -1.518824000 | 1.129451000 |
| Ag | -2.155933000 | -1.271854000 | -1.317787000 |
| Ag | 2.465738000 | 0.141880000 | -1.350728000 |
| Ag | -2.585443000 | 0.021403000 | 1.173265000 |
| Ag | 2.071527000 | 1.422457000 | 1.154205000 |
| Ag | -0.108809000 | 0.107371000 | -2.874306000 |
| Ag | -0.759833000 | 2.360870000 | 1.358928000 |
| Ag | 0.655417000 | -2.245729000 | -1.427762000 |
| Ag | -0.022849000 | -0.016654000 | 2.735817000 |
| Ag | 3.667144000 | 2.925381000 | -0.977109000 |
| S | 5.848997000 | 1.996189000 | -0.373447000 |
| Ag | 4.726202000 | 0.153045000 | 0.793551000 |
| C | 6.541835000 | 1.223418000 | -1.898515000 |
| H | 7.433598000 | 0.650817000 | -1.614177000 |
| H | 5.807587000 | 0.552745000 | -2.365379000 |
| H | 6.823914000 | 2.019085000 | -2.599328000 |
| Ag | -4.802844000 | 0.036141000 | -0.923235000 |
| S | -5.934538000 | -1.911228000 | 0.034415000 |
| Ag | -3.759161000 | -2.940653000 | 0.542444000 |
| C | -6.696923000 | -1.332707000 | 1.607527000 |
| H | -7.580071000 | -0.727075000 | 1.364799000 |
| H | -5.982196000 | -0.731443000 | 2.187052000 |
| H | -7.003800000 | -2.212550000 | 2.187336000 |
| Ag | -2.163501000 | 1.695261000 | 3.946106000 |
| S | -0.781078000 | 3.423123000 | 4.966970000 |
| Ag | 1.176559000 | 2.576401000 | 3.734991000 |
| C | -0.403486000 | 2.763971000 | 6.655278000 |
| H | 0.323004000 | 3.431142000 | 7.131733000 |
| H | 0.022415000 | 1.756945000 | 6.586122000 |
| H | -1.325961000 | 2.741576000 | 7.246535000 |
| Ag | -1.217142000 | -2.545507000 | -3.811808000 |
| S | 0.463155000 | -3.081636000 | -5.539138000 |
| Ag | 2.007369000 | -1.973598000 | -3.999448000 |
| C | 0.182158000 | -1.861486000 | -6.894029000 |
| H | 1.028531000 | -1.917144000 | -7.589604000 |
| H | 0.110214000 | -0.842020000 | -6.494690000 |
| H | -0.742875000 | -2.123874000 | -7.420886000 |
| Ag | 1.241972000 | -4.449386000 | 0.792915000 |
| S | 1.396728000 | -5.011444000 | 3.192014000 |
| Ag | 0.866467000 | -2.666448000 | 3.684409000 |
| C | 3.215072000 | -5.081297000 | 3.504331000 |
| H | 3.392339000 | -5.049500000 | 4.587059000 |
| H | 3.723878000 | -4.239599000 | 3.014079000 |

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|----|--------------|--------------|--------------|
| H | 3.596825000 | -6.024858000 | 3.095918000 |
| Ag | -0.755867000 | 3.017263000 | -3.709656000 |
| S | -1.607165000 | 5.286469000 | -3.259813000 |
| Ag | -1.342410000 | 4.576417000 | -0.907532000 |
| C | -3.425873000 | 5.226480000 | -3.561489000 |
| H | -3.887215000 | 6.090695000 | -3.066826000 |
| H | -3.856662000 | 4.298062000 | -3.159836000 |
| H | -3.604510000 | 5.282416000 | -4.643517000 |
| S | -3.244634000 | -3.238536000 | -2.526325000 |
| S | -3.958542000 | 0.182895000 | 3.292968000 |
| S | 3.998371000 | -1.152569000 | -2.851062000 |
| S | 3.527645000 | 2.300289000 | 3.030127000 |
| S | -4.310548000 | 1.942749000 | -2.386593000 |
| S | -2.020194000 | -4.566618000 | 1.151395000 |
| S | 1.975975000 | 4.690607000 | -1.292384000 |
| S | 4.279538000 | -1.925126000 | 2.015117000 |
| S | 1.377533000 | -4.620294000 | -1.649019000 |
| S | 0.712960000 | -0.610817000 | 5.101884000 |
| S | 0.365788000 | 1.274925000 | -5.069817000 |
| S | -1.358134000 | 4.758974000 | 1.542919000 |
| C | -0.835310000 | -0.841274000 | 6.088352000 |
| H | -1.293669000 | -1.810538000 | 5.875918000 |
| H | -0.568461000 | -0.791221000 | 7.150924000 |
| H | -1.554543000 | -0.042592000 | 5.853002000 |
| C | -0.226578000 | -5.438250000 | -2.067719000 |
| H | -1.031373000 | -5.080575000 | -1.418210000 |
| H | -0.109328000 | -6.519472000 | -1.932474000 |
| H | -0.469973000 | -5.216114000 | -3.112608000 |
| C | 0.303917000 | 5.494335000 | 1.878563000 |
| H | 1.042470000 | 5.126652000 | 1.157601000 |
| H | 0.224962000 | 6.584507000 | 1.784541000 |
| H | 0.599229000 | 5.225510000 | 2.899751000 |
| C | 2.156132000 | 1.639242000 | -4.781426000 |
| H | 2.349975000 | 1.866963000 | -3.723517000 |
| H | 2.458780000 | 2.489120000 | -5.404203000 |
| H | 2.743039000 | 0.754900000 | -5.056781000 |
| C | 4.053401000 | 3.959229000 | 2.401816000 |
| H | 3.279242000 | 4.413196000 | 1.775221000 |
| H | 4.263690000 | 4.614603000 | 3.254243000 |
| H | 4.963567000 | 3.823400000 | 1.805066000 |
| C | 4.430948000 | -2.540946000 | -1.710541000 |
| H | 3.572763000 | -2.817285000 | -1.087689000 |
| H | 4.746701000 | -3.409342000 | -2.296086000 |
| H | 5.246906000 | -2.204176000 | -1.059196000 |
| C | -3.486520000 | -1.494088000 | 3.905286000 |
| H | -2.429409000 | -1.701037000 | 3.690746000 |
| H | -3.669172000 | -1.560898000 | 4.985131000 |
| H | -4.101511000 | -2.234572000 | 3.369499000 |
| C | -4.713816000 | -2.508104000 | -3.370506000 |
| H | -4.588182000 | -1.433357000 | -3.535664000 |
| H | -4.861809000 | -3.009620000 | -4.334114000 |
| H | -5.588995000 | -2.669348000 | -2.729233000 |
| C | 4.073501000 | -1.279198000 | 3.736084000 |
| H | 3.510662000 | -0.338999000 | 3.743813000 |
| H | 5.064538000 | -1.105151000 | 4.170439000 |
| H | 3.532676000 | -2.027358000 | 4.329992000 |

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|---|--------------|--------------|--------------|
| C | -2.177693000 | -4.905261000 | 2.959400000 |
| H | -2.311295000 | -3.976712000 | 3.524247000 |
| H | -3.041630000 | -5.560975000 | 3.122988000 |
| H | -1.261029000 | -5.404669000 | 3.297680000 |
| C | 2.026327000 | 5.138076000 | -3.084284000 |
| H | 1.970209000 | 4.246509000 | -3.718462000 |
| H | 2.954885000 | 5.682044000 | -3.295461000 |
| H | 1.160266000 | 5.779065000 | -3.294658000 |
| C | -3.780250000 | 1.150473000 | -3.973531000 |
| H | -3.070118000 | 0.329471000 | -3.796539000 |
| H | -4.657468000 | 0.773029000 | -4.512254000 |
| H | -3.277319000 | 1.915911000 | -4.580841000 |

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Ag25(SeMe)18- S0 Ground State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.032239000 | 0.053495000 | 0.003779000 |
| Ag | -2.068222000 | 1.604598000 | -1.129548000 |
| Ag | -0.689430000 | -2.400210000 | 1.215557000 |
| Ag | 0.626295000 | 2.479237000 | -1.185622000 |
| Ag | 1.998054000 | -1.514194000 | 1.129287000 |
| Ag | -2.152771000 | -1.369181000 | -1.184792000 |
| Ag | 2.420849000 | 0.178880000 | -1.316612000 |
| Ag | -2.544747000 | -0.021257000 | 1.253400000 |
| Ag | 2.059573000 | 1.434137000 | 1.211939000 |
| Ag | -0.183066000 | -0.010266000 | -2.789400000 |
| Ag | -0.778690000 | 2.355376000 | 1.414280000 |
| Ag | 0.719148000 | -2.267457000 | -1.389337000 |
| Ag | 0.026002000 | -0.008920000 | 2.788043000 |
| Ag | 3.615608000 | 3.019407000 | -0.688079000 |
| Se | 5.878203000 | 2.156144000 | 0.177885000 |
| Ag | 4.621280000 | -0.012681000 | 0.777869000 |
| C | 6.802489000 | 1.687928000 | -1.547943000 |
| H | 7.606847000 | 0.983372000 | -1.316002000 |
| H | 6.073886000 | 1.237560000 | -2.232084000 |
| H | 7.207890000 | 2.610908000 | -1.974026000 |
| Ag | -4.748408000 | 0.160223000 | -0.743540000 |
| Se | -5.993378000 | -2.032887000 | -0.175225000 |
| Ag | -3.746485000 | -2.949902000 | 0.696694000 |
| C | -7.068452000 | -1.413481000 | 1.413217000 |
| H | -7.922964000 | -0.841664000 | 1.038463000 |
| H | -6.431343000 | -0.782999000 | 2.044591000 |
| H | -7.402293000 | -2.303810000 | 1.954755000 |
| Ag | -2.327023000 | 1.728682000 | 3.866168000 |
| Se | -0.907974000 | 3.568349000 | 4.980917000 |
| Ag | 1.139345000 | 2.507601000 | 3.806827000 |
| C | -0.439277000 | 2.936240000 | 6.848617000 |
| H | 0.256246000 | 3.666324000 | 7.272775000 |
| H | 0.036758000 | 1.952461000 | 6.795841000 |
| H | -1.364439000 | 2.895480000 | 7.431231000 |
| Ag | -1.100847000 | -2.878243000 | -3.608859000 |
| Se | 0.820461000 | -3.452680000 | -5.225375000 |
| Ag | 2.130902000 | -1.666255000 | -3.913793000 |
| C | 0.169299000 | -2.495686000 | -6.872924000 |
| H | 1.025350000 | -2.332498000 | -7.534719000 |
| H | -0.284649000 | -1.543000000 | -6.574144000 |
| H | -0.576275000 | -3.135696000 | -7.355023000 |
| Ag | 1.569261000 | -4.368194000 | 0.695596000 |

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|----|--------------|--------------|--------------|
| Se | 1.189117000 | -5.071292000 | 3.168030000 |
| Ag | 1.011992000 | -2.579669000 | 3.763638000 |
| C | 3.077417000 | -5.421643000 | 3.770489000 |
| H | 3.148550000 | -5.240881000 | 4.847718000 |
| H | 3.750907000 | -4.763905000 | 3.211767000 |
| H | 3.299397000 | -6.468952000 | 3.540225000 |
| Ag | -0.988529000 | 2.830343000 | -3.689475000 |
| Se | -1.287267000 | 5.319930000 | -3.115350000 |
| Ag | -1.592260000 | 4.496323000 | -0.682079000 |
| C | -3.196596000 | 5.538023000 | -3.731863000 |
| H | -3.504823000 | 6.554398000 | -3.473081000 |
| H | -3.813619000 | 4.808467000 | -3.197994000 |
| H | -3.240597000 | 5.382132000 | -4.812451000 |
| Se | -3.345024000 | -3.402635000 | -2.445862000 |
| Se | -4.373120000 | 0.374399000 | 3.107257000 |
| Se | 4.146164000 | -0.190613000 | -3.249549000 |
| Se | 3.626841000 | 1.950798000 | 3.321394000 |
| Se | -4.447170000 | 2.521133000 | -1.799656000 |
| Se | -1.990955000 | -4.691786000 | 1.401425000 |
| Se | 1.890548000 | 4.800999000 | -1.411549000 |
| Se | 4.395419000 | -2.456447000 | 1.658277000 |
| Se | 2.059788000 | -4.521186000 | -1.833733000 |
| Se | 1.005316000 | -0.426610000 | 5.238976000 |
| Se | -0.769475000 | 0.758253000 | -5.237251000 |
| Se | -1.767659000 | 4.764102000 | 1.872313000 |
| C | -0.767846000 | -0.663608000 | 6.214622000 |
| H | -1.282262000 | -1.543126000 | 5.828104000 |
| H | -0.532298000 | -0.787661000 | 7.275052000 |
| H | -1.369077000 | 0.236092000 | 6.042351000 |
| C | 0.515294000 | -5.772735000 | -2.247289000 |
| H | -0.388060000 | -5.406677000 | -1.751728000 |
| H | 0.785998000 | -6.763029000 | -1.869236000 |
| H | 0.384160000 | -5.780121000 | -3.332638000 |
| C | 0.054827000 | 5.648422000 | 2.044968000 |
| H | 0.793405000 | 5.070630000 | 1.479369000 |
| H | -0.021407000 | 6.662977000 | 1.643167000 |
| H | 0.304433000 | 5.653470000 | 3.110140000 |
| C | 1.122645000 | 1.058820000 | -5.890823000 |
| H | 1.744541000 | 1.394798000 | -5.057423000 |
| H | 1.093278000 | 1.809461000 | -6.686615000 |
| H | 1.487534000 | 0.097628000 | -6.265842000 |
| C | 4.345867000 | 3.812671000 | 2.956342000 |
| H | 3.807298000 | 4.236892000 | 2.109522000 |
| H | 4.191900000 | 4.413564000 | 3.853399000 |
| H | 5.405063000 | 3.708866000 | 2.722254000 |
| C | 5.174904000 | -1.676606000 | -2.321468000 |
| H | 4.472373000 | -2.309729000 | -1.773912000 |
| H | 5.696588000 | -2.250253000 | -3.092473000 |
| H | 5.877711000 | -1.203309000 | -1.629841000 |
| C | -3.942634000 | -1.397657000 | 3.993613000 |
| H | -2.876019000 | -1.599716000 | 3.876835000 |
| H | -4.217738000 | -1.328755000 | 5.048352000 |
| H | -4.526433000 | -2.172577000 | 3.484162000 |
| C | -4.583126000 | -2.312296000 | -3.631000000 |
| H | -4.147498000 | -1.327263000 | -3.810501000 |
| H | -4.707887000 | -2.855851000 | -4.569613000 |

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|---|--------------|--------------|--------------|
| H | -5.532995000 | -2.215373000 | -3.100753000 |
| C | 4.507793000 | -1.947480000 | 3.620822000 |
| H | 4.131700000 | -0.929573000 | 3.750716000 |
| H | 5.558980000 | -2.007856000 | 3.913671000 |
| H | 3.897464000 | -2.655835000 | 4.189632000 |
| C | -2.398947000 | -4.849304000 | 3.395973000 |
| H | -2.315997000 | -3.863662000 | 3.857265000 |
| H | -3.414604000 | -5.238508000 | 3.494513000 |
| H | -1.658299000 | -5.533015000 | 3.813472000 |
| C | 2.331770000 | 4.754807000 | -3.396448000 |
| H | 2.336323000 | 3.719829000 | -3.748388000 |
| H | 3.313616000 | 5.216693000 | -3.533383000 |
| H | 1.546967000 | 5.325006000 | -3.902107000 |
| C | -4.383357000 | 1.888344000 | -3.726395000 |
| H | -3.781802000 | 0.977114000 | -3.791002000 |
| H | -5.408947000 | 1.700130000 | -4.057623000 |
| H | -3.919133000 | 2.682635000 | -4.319617000 |

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Ag25 (SeMe)18- S1 Excited State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.029509000 | 0.083591000 | 0.073523000 |
| Ag | -2.059759000 | 1.613915000 | -1.124402000 |
| Ag | -0.815926000 | -2.343633000 | 1.305083000 |
| Ag | 0.692330000 | 2.525981000 | -1.140189000 |
| Ag | 1.977263000 | -1.474215000 | 1.248565000 |
| Ag | -2.129104000 | -1.288148000 | -1.235073000 |
| Ag | 2.437712000 | 0.258681000 | -1.241301000 |
| Ag | -2.574011000 | -0.012992000 | 1.273826000 |
| Ag | 2.070780000 | 1.422294000 | 1.333955000 |
| Ag | -0.096930000 | 0.172716000 | -2.707765000 |
| Ag | -0.780044000 | 2.397010000 | 1.472437000 |
| Ag | 0.728790000 | -2.247693000 | -1.303467000 |
| Ag | -0.042321000 | -0.059062000 | 2.856769000 |
| Ag | 3.747204000 | 2.982137000 | -0.459848000 |
| Se | 6.020912000 | 2.012203000 | 0.259675000 |
| Ag | 4.602241000 | -0.087642000 | 0.814114000 |
| C | 6.828020000 | 1.588431000 | -1.539330000 |
| H | 7.556271000 | 0.783628000 | -1.403330000 |
| H | 6.029242000 | 1.285527000 | -2.225420000 |
| H | 7.316877000 | 2.498299000 | -1.901611000 |
| Ag | -4.733063000 | 0.369333000 | -0.671492000 |
| Se | -5.988703000 | -1.845491000 | -0.251723000 |
| Ag | -3.773689000 | -2.912269000 | 0.503709000 |
| C | -6.963944000 | -1.347038000 | 1.442454000 |
| H | -7.769545000 | -0.654871000 | 1.179944000 |
| H | -6.253595000 | -0.874782000 | 2.130371000 |
| H | -7.366292000 | -2.270466000 | 1.870774000 |
| Ag | -2.233294000 | 1.725719000 | 3.948145000 |
| Se | -0.900322000 | 3.748638000 | 4.827746000 |
| Ag | 1.128289000 | 2.472927000 | 3.854815000 |
| C | -0.510431000 | 3.154206000 | 6.727167000 |
| H | 0.214050000 | 3.857817000 | 7.148332000 |
| H | -0.086628000 | 2.145716000 | 6.699501000 |
| H | -1.447087000 | 3.172257000 | 7.292296000 |
| Ag | -0.949136000 | -2.523109000 | -3.682549000 |
| Se | 1.003752000 | -3.619447000 | -5.061212000 |
| Ag | 2.016226000 | -1.539909000 | -3.916785000 |

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|----|--------------|--------------|--------------|
| C | 0.316756000 | -2.952654000 | -6.848381000 |
| H | 1.165973000 | -2.654905000 | -7.469804000 |
| H | -0.360541000 | -2.110831000 | -6.679444000 |
| H | -0.227053000 | -3.784499000 | -7.306826000 |
| Ag | 1.342510000 | -4.352641000 | 1.157677000 |
| Se | 1.079044000 | -5.192509000 | 3.633334000 |
| Ag | 0.890439000 | -2.591276000 | 3.782861000 |
| C | 3.046410000 | -5.443753000 | 4.041257000 |
| H | 3.240366000 | -5.100445000 | 5.061330000 |
| H | 3.633588000 | -4.873925000 | 3.315393000 |
| H | 3.258222000 | -6.513451000 | 3.944778000 |
| Ag | -1.008618000 | 2.670384000 | -3.630133000 |
| Se | -1.092911000 | 5.291576000 | -3.679678000 |
| Ag | -1.434813000 | 4.533556000 | -1.190514000 |
| C | -3.041503000 | 5.614640000 | -4.129558000 |
| H | -3.215354000 | 6.693255000 | -4.061537000 |
| H | -3.664783000 | 5.085774000 | -3.402682000 |
| H | -3.230229000 | 5.255352000 | -5.145390000 |
| Se | -3.316196000 | -3.136939000 | -2.736189000 |
| Se | -4.107184000 | 0.053818000 | 3.413414000 |
| Se | 3.971992000 | 0.054091000 | -3.333074000 |
| Se | 3.599371000 | 1.667612000 | 3.515823000 |
| Se | -4.393896000 | 2.796610000 | -1.571951000 |
| Se | -1.945665000 | -4.695443000 | 0.841570000 |
| Se | 1.999426000 | 4.823027000 | -0.864568000 |
| Se | 4.348261000 | -2.576735000 | 1.581230000 |
| Se | 2.137300000 | -4.442572000 | -1.319388000 |
| Se | 0.984927000 | -0.376750000 | 5.321862000 |
| Se | -1.330192000 | 0.358763000 | -5.077035000 |
| Se | -2.053006000 | 4.673277000 | 1.319890000 |
| C | -0.733234000 | -0.635467000 | 6.365581000 |
| H | -1.123857000 | -1.638989000 | 6.181942000 |
| H | -0.490865000 | -0.506555000 | 7.424907000 |
| H | -1.458219000 | 0.120229000 | 6.038068000 |
| C | 0.659495000 | -5.667063000 | -1.973750000 |
| H | -0.254215000 | -5.440998000 | -1.416171000 |
| H | 0.984583000 | -6.692961000 | -1.774812000 |
| H | 0.518375000 | -5.489782000 | -3.043378000 |
| C | -0.488922000 | 5.853519000 | 1.844913000 |
| H | 0.416077000 | 5.463872000 | 1.370695000 |
| H | -0.703126000 | 6.862086000 | 1.479382000 |
| H | -0.404016000 | 5.827550000 | 2.934787000 |
| C | 0.347263000 | 0.631958000 | -6.185336000 |
| H | 0.965911000 | 1.394479000 | -5.707328000 |
| H | 0.036814000 | 0.948695000 | -7.185753000 |
| H | 0.891609000 | -0.316849000 | -6.224129000 |
| C | 4.542322000 | 3.428225000 | 3.175233000 |
| H | 4.105033000 | 3.906694000 | 2.294140000 |
| H | 4.416099000 | 4.054920000 | 4.062305000 |
| H | 5.597904000 | 3.202122000 | 2.998546000 |
| C | 5.083507000 | -1.467875000 | -2.562581000 |
| H | 4.410560000 | -2.212707000 | -2.128398000 |
| H | 5.667101000 | -1.900757000 | -3.379992000 |
| H | 5.729311000 | -1.042807000 | -1.788285000 |
| C | -3.370978000 | -1.703229000 | 4.097202000 |
| H | -2.294876000 | -1.747467000 | 3.897002000 |

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|---|--------------|--------------|--------------|
| H | -3.574901000 | -1.766296000 | 5.170039000 |
| H | -3.885465000 | -2.497677000 | 3.546806000 |
| C | -4.394080000 | -1.774267000 | -3.779979000 |
| H | -3.735250000 | -0.952991000 | -4.076207000 |
| H | -4.792467000 | -2.275939000 | -4.667298000 |
| H | -5.202896000 | -1.415111000 | -3.135709000 |
| C | 4.492439000 | -2.146251000 | 3.558497000 |
| H | 4.409530000 | -1.064585000 | 3.700064000 |
| H | 5.466838000 | -2.508516000 | 3.900300000 |
| H | 3.677666000 | -2.659772000 | 4.078353000 |
| C | -2.273874000 | -5.241325000 | 2.763533000 |
| H | -2.047551000 | -4.396385000 | 3.419581000 |
| H | -3.321719000 | -5.539253000 | 2.858718000 |
| H | -1.602398000 | -6.077768000 | 2.979465000 |
| C | 2.357806000 | 5.041213000 | -2.849701000 |
| H | 2.284496000 | 4.064199000 | -3.334582000 |
| H | 3.358633000 | 5.463339000 | -2.973826000 |
| H | 1.590336000 | 5.717169000 | -3.239385000 |
| C | -4.551860000 | 2.267899000 | -3.524977000 |
| H | -4.224640000 | 1.233862000 | -3.650615000 |
| H | -5.600715000 | 2.378752000 | -3.816843000 |
| H | -3.907649000 | 2.932391000 | -4.108497000 |

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Ag25(TeMe)18- S0 Ground State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.016690000 | 0.041455000 | 0.065368000 |
| Ag | -2.150308000 | 1.463119000 | -1.014214000 |
| Ag | -0.696093000 | -2.465641000 | 1.173532000 |
| Ag | 0.639827000 | 2.548695000 | -1.026511000 |
| Ag | 2.105146000 | -1.392099000 | 1.131276000 |
| Ag | -2.009306000 | -1.448953000 | -1.237692000 |
| Ag | 2.385290000 | 0.244336000 | -1.298766000 |
| Ag | -2.451152000 | -0.133112000 | 1.392052000 |
| Ag | 1.960310000 | 1.523682000 | 1.350348000 |
| Ag | -0.143814000 | 0.209951000 | -2.696731000 |
| Ag | -0.864391000 | 2.321013000 | 1.473506000 |
| Ag | 0.832472000 | -2.235496000 | -1.316191000 |
| Ag | 0.037000000 | -0.191895000 | 2.825700000 |
| Ag | 3.813229000 | 2.720564000 | -0.764276000 |
| Te | 6.369566000 | 2.315377000 | 0.343302000 |
| Ag | 4.550886000 | 0.261860000 | 0.837227000 |
| C | 7.444338000 | 1.788005000 | -1.531297000 |
| H | 8.031902000 | 0.884901000 | -1.347749000 |
| H | 6.696601000 | 1.622886000 | -2.314968000 |
| H | 8.085657000 | 2.636396000 | -1.781920000 |
| Ag | -4.655641000 | 0.005926000 | -0.459946000 |
| Te | -6.180971000 | -2.312112000 | -0.327988000 |
| Ag | -3.645723000 | -2.886621000 | 0.666237000 |
| C | -7.415124000 | -1.697921000 | 1.430242000 |
| H | -8.290962000 | -1.168378000 | 1.048807000 |
| H | -6.802388000 | -1.035379000 | 2.049386000 |
| H | -7.700723000 | -2.601597000 | 1.974035000 |
| Ag | -2.160420000 | 1.552116000 | 3.962318000 |
| Te | -1.055076000 | 3.506068000 | 5.577166000 |
| Ag | 0.914581000 | 2.319658000 | 3.994946000 |
| C | -0.642918000 | 2.362319000 | 7.455376000 |
| H | -0.102154000 | 3.029793000 | 8.135043000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -0.019146000 | 1.502671000 | 7.188675000 |
| H | -1.598440000 | 2.044344000 | 7.882083000 |
| Ag | -0.784996000 | -2.406546000 | -3.818880000 |
| Te | 1.237122000 | -3.369365000 | -5.525763000 |
| Ag | 2.117211000 | -1.343379000 | -3.840672000 |
| C | 0.535927000 | -2.337395000 | -7.375101000 |
| H | 1.392049000 | -1.858662000 | -7.860878000 |
| H | -0.220989000 | -1.600941000 | -7.082861000 |
| H | 0.091953000 | -3.106380000 | -8.016723000 |
| Ag | 1.704968000 | -4.266514000 | 0.865457000 |
| Te | 1.594566000 | -5.589199000 | 3.341998000 |
| Ag | 1.070581000 | -2.861352000 | 3.531782000 |
| C | 3.713896000 | -5.504525000 | 4.031780000 |
| H | 3.732280000 | -5.154617000 | 5.066096000 |
| H | 4.245810000 | -4.818359000 | 3.364764000 |
| H | 4.118757000 | -6.516907000 | 3.946500000 |
| Ag | -1.173043000 | 2.821662000 | -3.463056000 |
| Te | -1.377260000 | 5.555177000 | -3.193565000 |
| Ag | -1.721188000 | 4.327485000 | -0.698311000 |
| C | -3.514195000 | 5.800986000 | -3.800028000 |
| H | -3.745108000 | 6.866441000 | -3.722619000 |
| H | -4.125483000 | 5.227196000 | -3.097829000 |
| H | -3.638237000 | 5.439870000 | -4.822615000 |
| Te | -3.368134000 | -3.158662000 | -2.989776000 |
| Te | -4.526637000 | 0.290028000 | 3.204854000 |
| Te | 4.304597000 | 0.339485000 | -3.309613000 |
| Te | 3.676141000 | 2.293370000 | 3.435986000 |
| Te | -4.622155000 | 2.730898000 | -1.285451000 |
| Te | -1.931086000 | -4.948488000 | 1.486558000 |
| Te | 2.210332000 | 4.619763000 | -2.043439000 |
| Te | 4.607181000 | -2.411764000 | 1.761590000 |
| Te | 1.894113000 | -4.733649000 | -1.882733000 |
| Te | 0.925414000 | -0.758890000 | 5.416892000 |
| Te | -1.217949000 | 0.641891000 | -5.249469000 |
| Te | -1.506868000 | 4.965298000 | 2.025985000 |
| C | -1.149916000 | -1.106868000 | 6.175500000 |
| H | -1.552343000 | -1.987546000 | 5.673338000 |
| H | -1.072999000 | -1.258812000 | 7.254644000 |
| H | -1.738918000 | -0.212937000 | 5.941267000 |
| C | -0.152517000 | -5.604886000 | -2.108273000 |
| H | -0.827758000 | -5.042640000 | -1.458431000 |
| H | -0.100611000 | -6.653225000 | -1.807975000 |
| H | -0.426996000 | -5.486582000 | -3.160030000 |
| C | 0.675671000 | 5.430689000 | 1.922294000 |
| H | 1.143001000 | 4.706823000 | 1.249188000 |
| H | 0.788777000 | 6.449455000 | 1.541988000 |
| H | 1.061004000 | 5.321208000 | 2.939566000 |
| C | 0.746974000 | 0.988566000 | -6.248677000 |
| H | 1.239371000 | 1.819787000 | -5.741911000 |
| H | 0.542956000 | 1.219517000 | -7.296790000 |
| H | 1.326771000 | 0.067335000 | -6.141771000 |
| C | 4.028258000 | 4.374398000 | 2.693306000 |
| H | 3.574901000 | 4.463412000 | 1.701652000 |
| H | 3.569010000 | 5.058473000 | 3.409430000 |
| H | 5.113645000 | 4.499558000 | 2.638395000 |
| C | 5.490946000 | -1.231146000 | -2.252857000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.808380000 | -2.033829000 | -1.967554000 |
| H | 6.257884000 | -1.584790000 | -2.943829000 |
| H | 5.925112000 | -0.754993000 | -1.369660000 |
| C | -4.112506000 | -1.758820000 | 3.968866000 |
| H | -3.047856000 | -1.950688000 | 3.818404000 |
| H | -4.378729000 | -1.792213000 | 5.028997000 |
| H | -4.717524000 | -2.449633000 | 3.372607000 |
| C | -4.443920000 | -1.428159000 | -3.905263000 |
| H | -3.701516000 | -0.779153000 | -4.378940000 |
| H | -5.137124000 | -1.833603000 | -4.647906000 |
| H | -4.982955000 | -0.917163000 | -3.101955000 |
| C | 4.462217000 | -1.803210000 | 3.902543000 |
| H | 4.071236000 | -0.782652000 | 3.934811000 |
| H | 5.468674000 | -1.847387000 | 4.326137000 |
| H | 3.784048000 | -2.501934000 | 4.401303000 |
| C | -2.193755000 | -4.866855000 | 3.708422000 |
| H | -2.943096000 | -4.109976000 | 3.942113000 |
| H | -2.526441000 | -5.867019000 | 4.007219000 |
| H | -1.219418000 | -4.627875000 | 4.147609000 |
| C | 2.295915000 | 3.595609000 | -4.027886000 |
| H | 2.194987000 | 2.523118000 | -3.845018000 |
| H | 3.259678000 | 3.830915000 | -4.485837000 |
| H | 1.458373000 | 3.984110000 | -4.614359000 |
| C | -4.692707000 | 2.383198000 | -3.488925000 |
| H | -4.562396000 | 1.315257000 | -3.670143000 |
| H | -5.663845000 | 2.732574000 | -3.845020000 |
| H | -3.875681000 | 2.956906000 | -3.935329000 |

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Ag25(SMe)18- S1 Excited State

| | | | |
|----|--------------|--------------|--------------|
| Ag | -0.049948000 | 0.035598000 | 0.068468000 |
| Ag | -2.153769000 | 1.526892000 | -1.002491000 |
| Ag | -0.752348000 | -2.467425000 | 1.160146000 |
| Ag | 0.627206000 | 2.539145000 | -1.014998000 |
| Ag | 2.042838000 | -1.461905000 | 1.131588000 |
| Ag | -2.108012000 | -1.345527000 | -1.269080000 |
| Ag | 2.380234000 | 0.266902000 | -1.269572000 |
| Ag | -2.518843000 | -0.163618000 | 1.368075000 |
| Ag | 2.002002000 | 1.417696000 | 1.385929000 |
| Ag | -0.154224000 | 0.298057000 | -2.694732000 |
| Ag | -0.830012000 | 2.240779000 | 1.554479000 |
| Ag | 0.738483000 | -2.196631000 | -1.392723000 |
| Ag | -0.012980000 | -0.283031000 | 2.849196000 |
| Ag | 3.807284000 | 2.717033000 | -0.623640000 |
| Te | 6.358977000 | 2.206932000 | 0.416497000 |
| Ag | 4.533582000 | 0.136808000 | 0.819309000 |
| C | 7.381772000 | 1.749551000 | -1.502877000 |
| H | 8.007265000 | 0.865189000 | -1.359983000 |
| H | 6.609875000 | 1.573416000 | -2.259006000 |
| H | 7.983489000 | 2.623894000 | -1.766706000 |
| Ag | -4.689191000 | 0.115797000 | -0.477968000 |
| Te | -6.281596000 | -2.159558000 | -0.331752000 |
| Ag | -3.733144000 | -2.839892000 | 0.548162000 |
| C | -7.416471000 | -1.476881000 | 1.463191000 |
| H | -8.181871000 | -0.777438000 | 1.120451000 |
| H | -6.707223000 | -0.978272000 | 2.132658000 |
| H | -7.858665000 | -2.356925000 | 1.936246000 |

| | | | |
|----|--------------|--------------|--------------|
| Ag | -2.089314000 | 1.503715000 | 4.080701000 |
| Te | -1.018896000 | 3.605464000 | 5.548314000 |
| Ag | 0.897279000 | 2.226669000 | 4.047948000 |
| C | -0.509259000 | 2.536861000 | 7.449812000 |
| H | 0.142897000 | 3.194213000 | 8.030902000 |
| H | 0.015052000 | 1.617604000 | 7.174894000 |
| H | -1.440915000 | 2.324888000 | 7.980228000 |
| Ag | -0.827811000 | -2.256105000 | -3.915205000 |
| Te | 1.180981000 | -3.374676000 | -5.553341000 |
| Ag | 2.058533000 | -1.333351000 | -3.876239000 |
| C | 0.524704000 | -2.306863000 | -7.400603000 |
| H | 1.400735000 | -1.855325000 | -7.873236000 |
| H | -0.212398000 | -1.552714000 | -7.111890000 |
| H | 0.072066000 | -3.060017000 | -8.050892000 |
| Ag | 1.549313000 | -4.313763000 | 0.989754000 |
| Te | 1.511231000 | -5.645156000 | 3.489033000 |
| Ag | 0.953154000 | -2.885191000 | 3.535765000 |
| C | 3.666728000 | -5.566703000 | 4.034479000 |
| H | 3.758332000 | -5.112741000 | 5.023545000 |
| H | 4.178954000 | -4.973488000 | 3.271745000 |
| H | 4.033190000 | -6.596753000 | 4.036406000 |
| Ag | -1.142936000 | 2.881062000 | -3.412449000 |
| Te | -1.401556000 | 5.670422000 | -3.407613000 |
| Ag | -1.601939000 | 4.409665000 | -0.884358000 |
| C | -3.557924000 | 5.828972000 | -3.978620000 |
| H | -3.801169000 | 6.895005000 | -3.993324000 |
| H | -4.139007000 | 5.308303000 | -3.212472000 |
| H | -3.694411000 | 5.375816000 | -4.963388000 |
| Te | -3.376493000 | -3.102653000 | -3.063349000 |
| Te | -4.392658000 | 0.132101000 | 3.426163000 |
| Te | 4.246010000 | 0.309177000 | -3.341682000 |
| Te | 3.658081000 | 2.193732000 | 3.525365000 |
| Te | -4.611078000 | 2.843502000 | -1.255786000 |
| Te | -2.015728000 | -4.958144000 | 1.216992000 |
| Te | 2.230323000 | 4.663398000 | -1.861646000 |
| Te | 4.545426000 | -2.541592000 | 1.706597000 |
| Te | 1.975859000 | -4.635414000 | -1.748828000 |
| Te | 0.881377000 | -0.756030000 | 5.485490000 |
| Te | -1.216975000 | 0.685573000 | -5.276790000 |
| Te | -1.507028000 | 4.889820000 | 1.861043000 |
| C | -1.136980000 | -1.043965000 | 6.397033000 |
| H | -1.599611000 | -1.917232000 | 5.933523000 |
| H | -0.983483000 | -1.193960000 | 7.469203000 |
| H | -1.720523000 | -0.138329000 | 6.199435000 |
| C | 0.047136000 | -5.637731000 | -2.251536000 |
| H | -0.596199000 | -5.573982000 | -1.370945000 |
| H | 0.284418000 | -6.676600000 | -2.495872000 |
| H | -0.374762000 | -5.106062000 | -3.109147000 |
| C | 0.651832000 | 5.430012000 | 1.990515000 |
| H | 1.130285000 | 5.107006000 | 1.062219000 |
| H | 0.713110000 | 6.515905000 | 2.115395000 |
| H | 1.055670000 | 4.897679000 | 2.857547000 |
| C | 0.779017000 | 1.050466000 | -6.201801000 |
| H | 1.269470000 | 1.847760000 | -5.639153000 |
| H | 0.609978000 | 1.340149000 | -7.242552000 |
| H | 1.345614000 | 0.115752000 | -6.130584000 |

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|---|--------------|--------------|--------------|
| C | 4.012867000 | 4.272380000 | 2.777477000 |
| H | 3.495155000 | 4.375388000 | 1.818730000 |
| H | 3.617660000 | 4.960758000 | 3.529534000 |
| H | 5.093897000 | 4.375086000 | 2.645685000 |
| C | 5.390313000 | -1.311841000 | -2.304687000 |
| H | 4.666173000 | -2.035542000 | -1.921026000 |
| H | 6.056595000 | -1.767316000 | -3.042045000 |
| H | 5.941567000 | -0.837780000 | -1.486873000 |
| C | -3.843576000 | -1.946258000 | 4.023215000 |
| H | -2.774651000 | -2.079848000 | 3.836939000 |
| H | -4.090165000 | -2.077636000 | 5.080112000 |
| H | -4.430166000 | -2.613173000 | 3.382994000 |
| C | -4.474006000 | -1.354954000 | -3.918139000 |
| H | -3.731819000 | -0.656933000 | -4.315176000 |
| H | -5.116703000 | -1.737075000 | -4.714566000 |
| H | -5.061355000 | -0.909297000 | -3.109993000 |
| C | 4.389791000 | -1.987177000 | 3.862860000 |
| H | 4.135685000 | -0.924145000 | 3.919911000 |
| H | 5.362293000 | -2.183835000 | 4.322401000 |
| H | 3.604943000 | -2.608271000 | 4.305438000 |
| C | -2.242687000 | -5.059331000 | 3.432842000 |
| H | -3.125661000 | -4.483054000 | 3.710904000 |
| H | -2.359162000 | -6.118741000 | 3.678983000 |
| H | -1.333946000 | -4.647500000 | 3.888516000 |
| C | 2.302529000 | 3.708287000 | -3.876428000 |
| H | 2.281907000 | 2.623723000 | -3.728268000 |
| H | 3.228619000 | 4.021210000 | -4.369784000 |
| H | 1.415572000 | 4.054495000 | -4.415593000 |
| C | -4.692345000 | 2.488636000 | -3.461047000 |
| H | -4.715567000 | 1.411315000 | -3.634033000 |
| H | -5.599083000 | 2.973842000 | -3.832583000 |
| H | -3.795883000 | 2.938050000 | -3.897410000 |