

Supporting Information

Regulating the Molecule and Electrode Interface of Single-Molecule Junction via Side Chain

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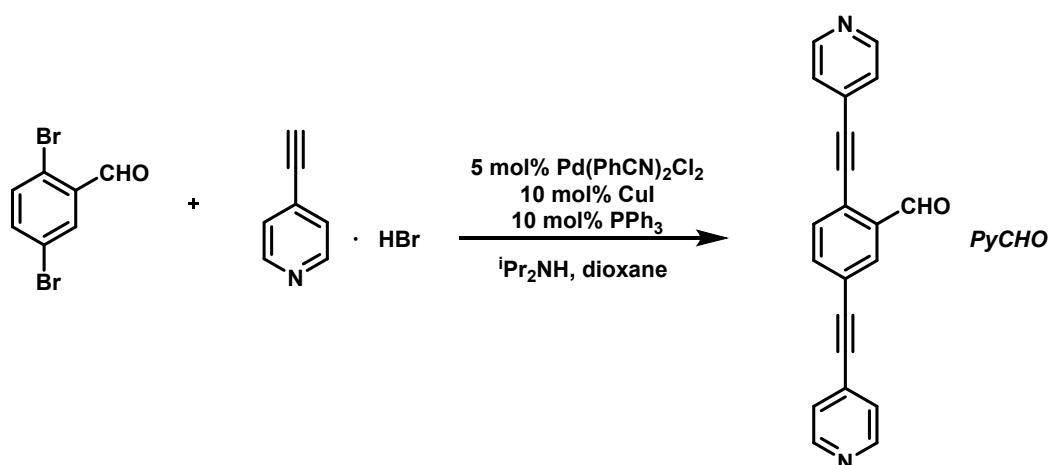
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General information

All available reagents and solvents were obtained from standard chemical suppliers and used without further purification unless mentioned. All reaction were carried out at Argon atmosphere and anhydrous conditions unless otherwise indicated. The column chromatography for purification was prepared with 200-300 mesh silica gel.

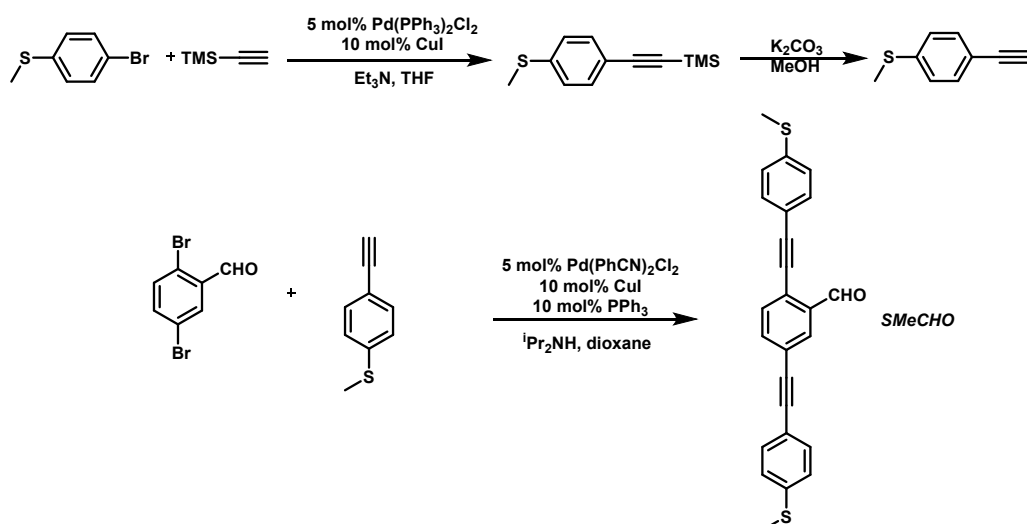
NMR spectra were recorded on a Bruker spectrometer and further analyzed with the MestReNova Software. High-resolution mass spectra (HRMS) were recorded on a GCT Premier mass spectrometer using EI-TOF (electron ionization-time of flight), Agilent Technologies 7250 GCQTOF (EI), and Xevo G2 TOF MS (ESI).

Experimental Section



Scheme S1 The synthesis of **PyCHO**

To a dried two-necked flask was added with 2,5-dibromobenzaldehyde (2.0 mmol, 0.524 g, 1.0 equiv.), 4-ethynylpyridine hydrobromic (5.0 mmol, 0.6979 g, 2.5 equiv.), $\text{Pd}(\text{PhCN})_2\text{Cl}_2$ (5 mol%, 40 mg), CuI (10 mol%, 14mg) and PPh_3 (10 mol%, 53 mg). The flask was degassed and backfilled with argon 3 times. After that, 10 mL $i\text{Pr}_2\text{NH}$ and 4 mL dioxane were added. The mixture was allowed to stir at 90°C overnight. The solution was quenched with water, extracted with DCM, dried with Na_2SO_4 , filtered and evaporated. The residue was purified by column chromatography on silica gel to give **PyCHO** as brown solid (0.5337g, 87%). ^1H NMR (400 MHz, CDCl_3): δ = 10.57 (s, 1H), 8.66 (dd, J = 11.6, 5.2 Hz, 4H), 8.13 (d, J = 1.6 Hz, 1H), 7.77 (dd, J = 8.0, 1.6 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.44 – 7.40 (m, 4H); ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$): δ = 191.0, 150.5, 137.1, 136.6, 134.8, 132.0, 130.0, 129.9, 126.0, 124.4, 123.2, 95.0, 92.1, 90.2, 89.5; HRMS(EI): $[\text{M}]^+$ Calcd for $\text{C}_{21}\text{H}_{12}\text{N}_2\text{O}$: 308.0950; found: 308.0954.



Scheme S2 The synthesis of **SMeCHO**

To a dried two-necked flask was charged with (4-bromophenyl)(methyl)sulfane (14.77 mmol, 3 g, 1.0 equiv.), Pd(PPh₃)₂Cl₂ (5 mol%, 0.519 g) and CuI (5 mol%, 0.141g). The flask was degassed and backfilled with argon 3 times. After that, ethynyltrimethylsilane (16.25 mmol, 1.6 g, 1.1 equiv) and Et₃N (60 mL) were added, the mixture stirred at 65°C overnight. Once the reaction completed, the solution was quenched with water, extracted with DCM, dried with Na₂SO₄, filtered and evaporated. The obtained solid was used for next step without further purification.

To a solution of TMS-protected (4-ethynylphenyl)(methyl)sulfane (8.01 mmol, 1.766g, 1.0 equiv) in THF was added with K₂CO₃ (40.06 mmol, 5.537 g, 5.0 equiv.), MeOH (15 mL), the mixture was allowed to stir at room temperature in darkness for 3 hours. When the starting materials were consumed monitored by TLC, the reaction was quenched by water, extracted by Et₂O, dried with Na₂SO₄, filtered and evaporated (**Caution: the temperature of evaporator should be below room temperature due to low boiling point of the products**). The solid was used for next step without further purification.

To a dried two-necked flask was added with 2,5-dibromobenzaldehyde (2.0 mmol, 0.524 g, 1.0 equiv.), (4-ethynylphenyl)(methyl)sulfane (5.0 mmol, 0.740 g, 2.5 equiv.), Pd(PhCN)₂Cl₂ (5 mol%, 40 mg), CuI (10 mol%, 14mg) and PPh₃ (10 mol%, 53 mg). The flask was degassed and backfilled with argon 3 times. After that, 10 mL *i*Pr₂NH and 4 mL dioxane were added, the mixture was allowed to stir at 90°C overnight. The solution was quenched with water, extracted with DCM, dried with Na₂SO₄, filtered and evaporated. The residue was purified by column chromatography on silica gel to give **SMeCHO** as brown solid (0.573g, 72%). ¹H NMR (400 MHz, CDCl₃): δ = 10.6 (s, 1H), 8.06 (d, *J* = 1.6 Hz, 1H), 7.68 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.42 (m, 4H), 7.25– 7.21 (m, 4H), 2.52 (s, 3H), 2.51 (s, 3H); ¹³C NMR (150 MHz, DMSO-*d*₆): δ = 191.3, 141.5, 141.0, 136.6, 136.0, 134.2, 132.4, 126.0, 126.0, 125.0, 123.4, 117.9, 117.7, 98.1, 92.8, 88.4, 85.9, 14.6; HRMS(EI): [M]⁺ Calcd for C₂₅H₁₈S₂O: 398.0799; found: 398.0802.

NMR and MS Spectra

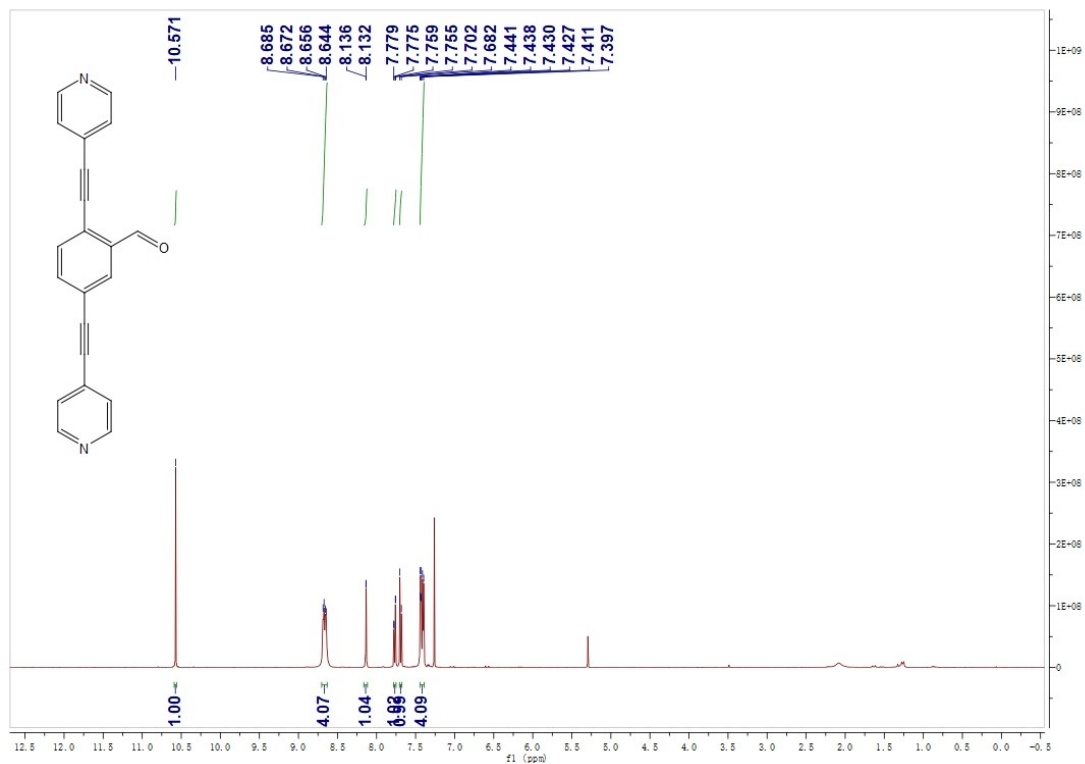


Figure S1. ^1H NMR-spectrum (400 MHz, CDCl_3) of PyCHO

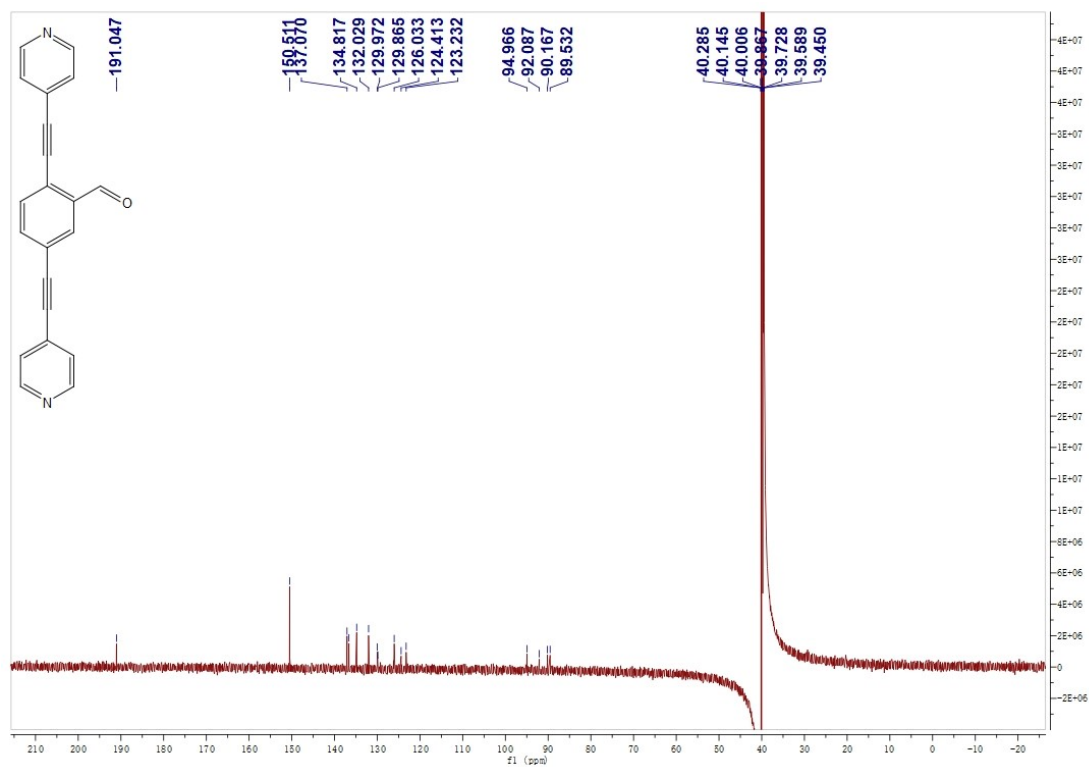


Figure S2. ^{13}C NMR-spectrum (150 MHz, DMSO-d_6) of PyCHO

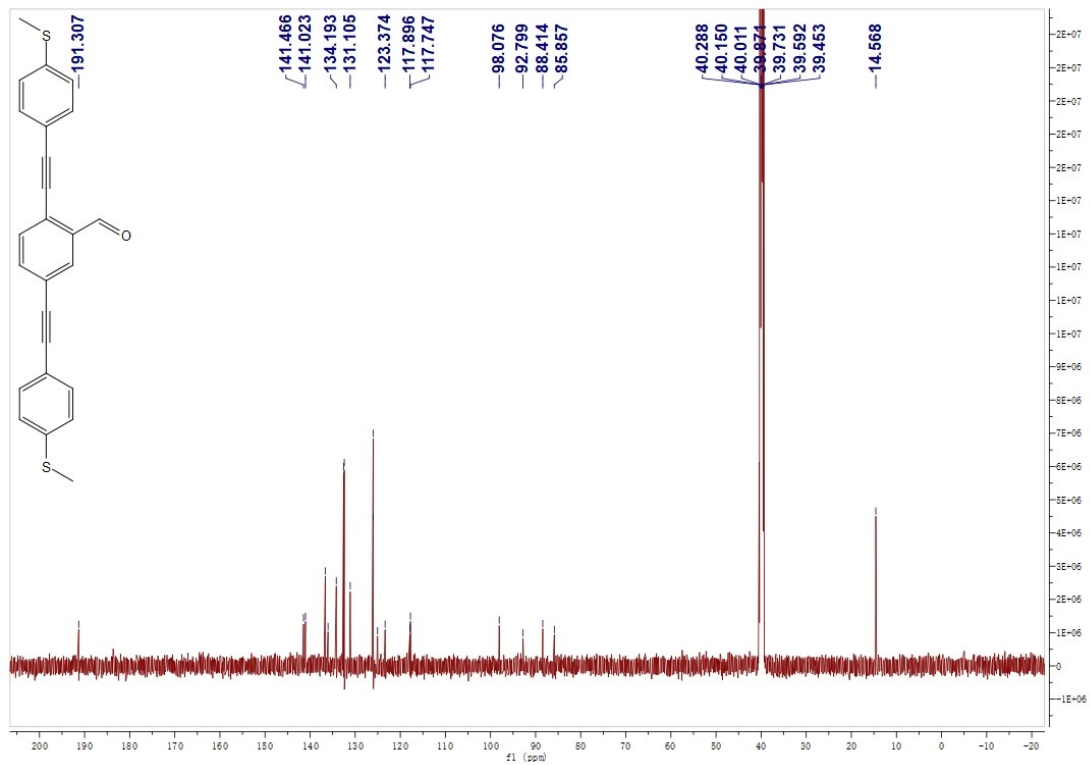


Figure S5. ^{13}C NMR-spectrum (150 MHz, DMSO-d_6) of SMeCHO

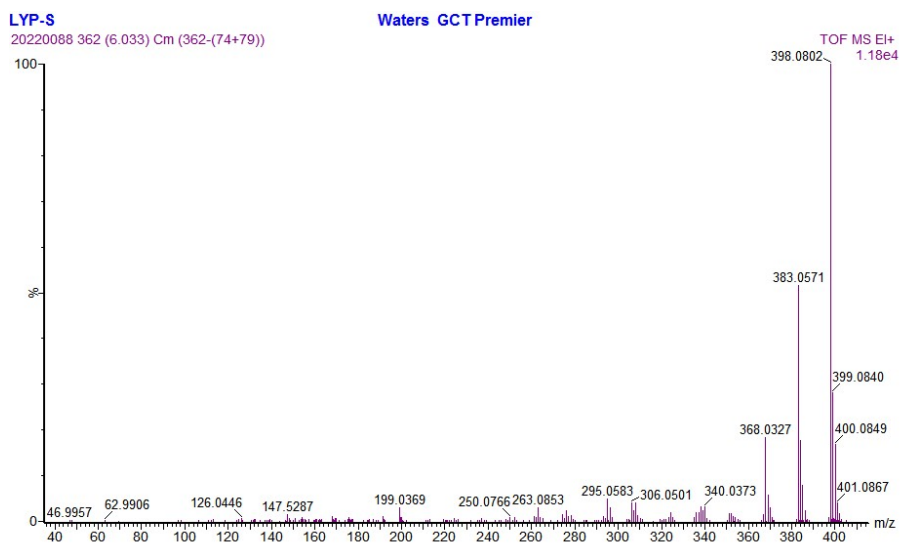


Figure S6. EI-MS-spectrum of SMeCHO

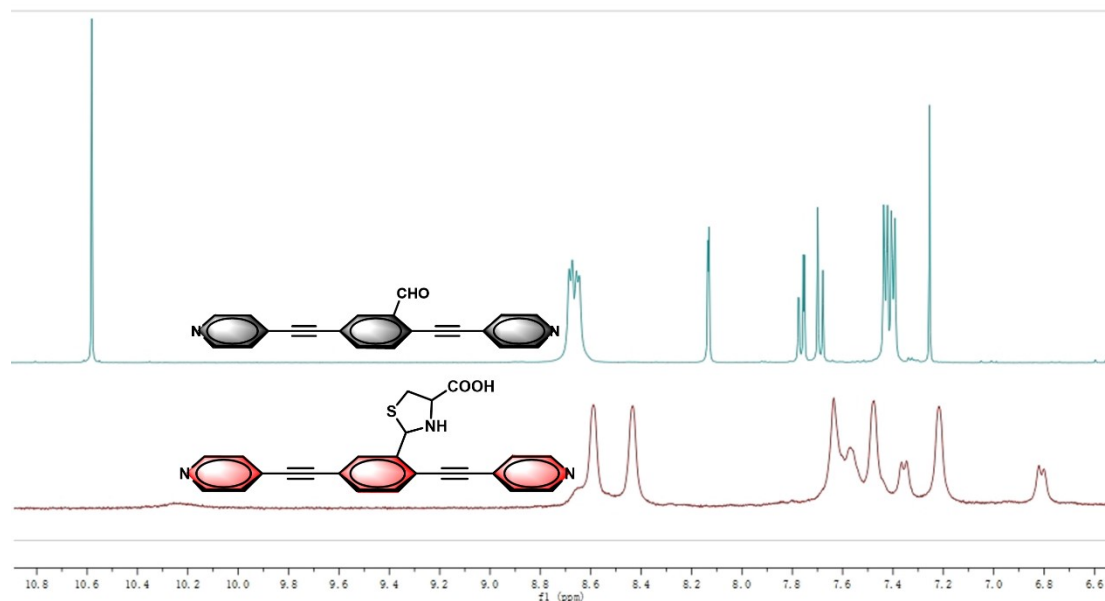


Figure S7. ¹H NMR spectrum of PyCHO (upper) and PyCHO+Cys (lower) in DMSO-*d*₆.

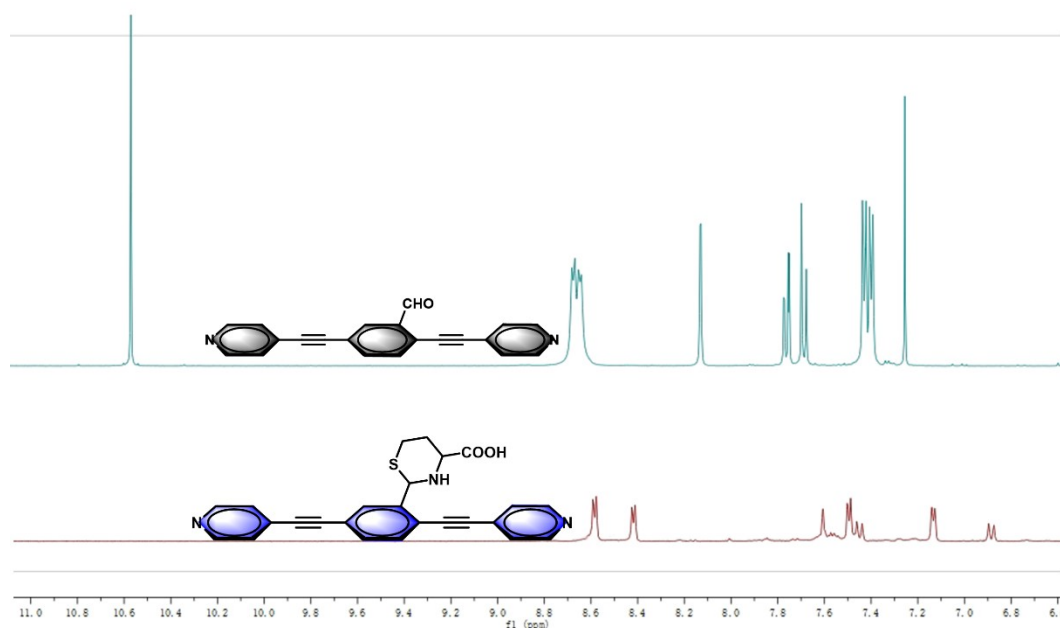


Figure S8. ¹H NMR spectrum of PyCHO (upper) and PyCHO+Hcy(lower) in DMSO-*d*₆.

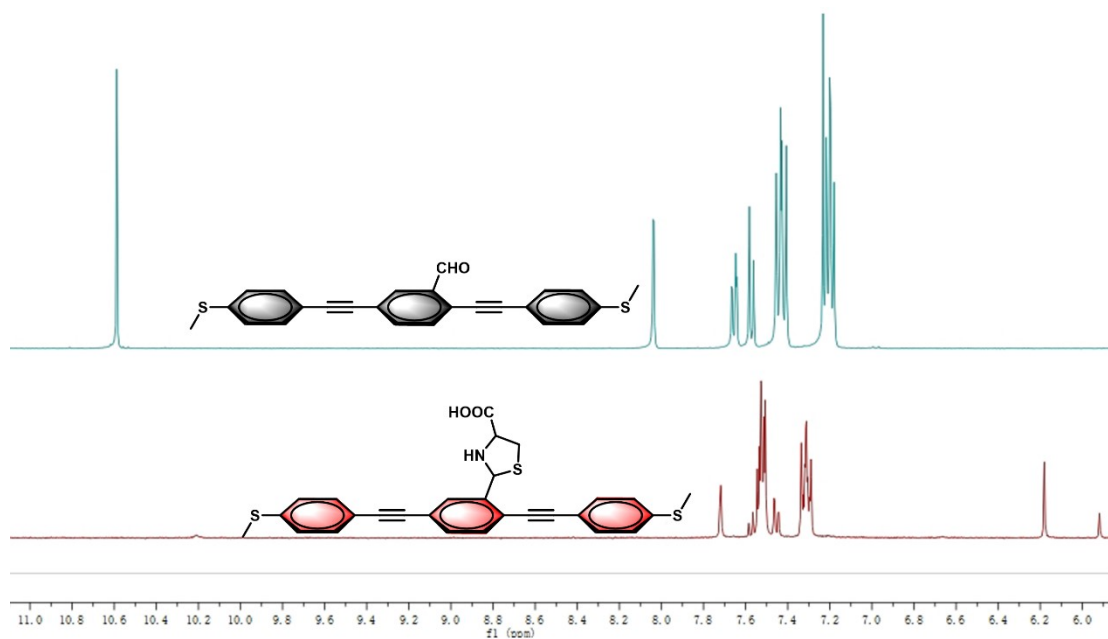


Figure S9. ¹H NMR spectrum of SMeCHO (upper) and SMeCHO+Cys(lower) in DMSO-*d*₆.

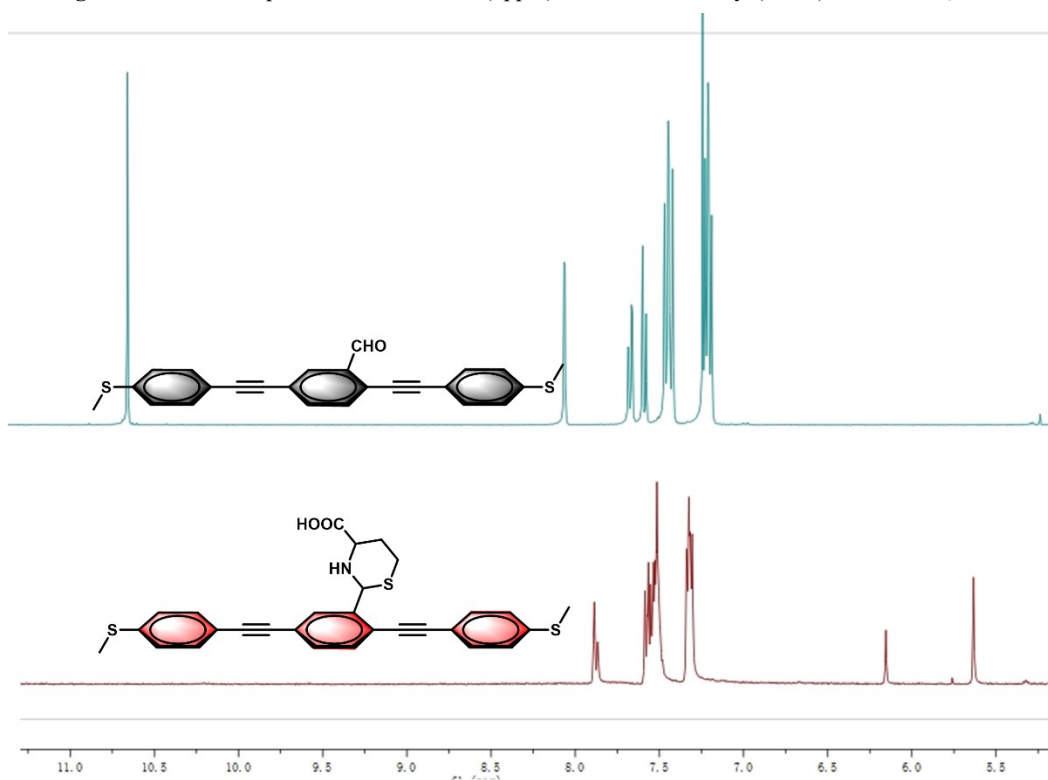


Figure S10. ¹H NMR spectrum of SMeCHO (upper) and SMeCHO+HCy(lower) in DMSO-*d*₆.

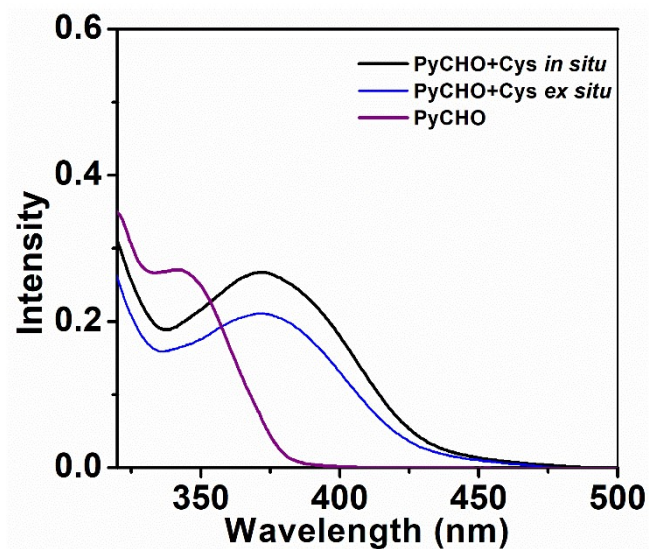


Figure S11. Absorption spectra PyCHO, PyCHO+Cys *in situ* and PyCHO+Cys *ex situ*. PyCHO+Cys *in situ* is the product prepared *in situ* by addition of 80 equiv. of Cys to a solution of PyCHO; PyCHO+Cys *ex situ* is the isolated product.

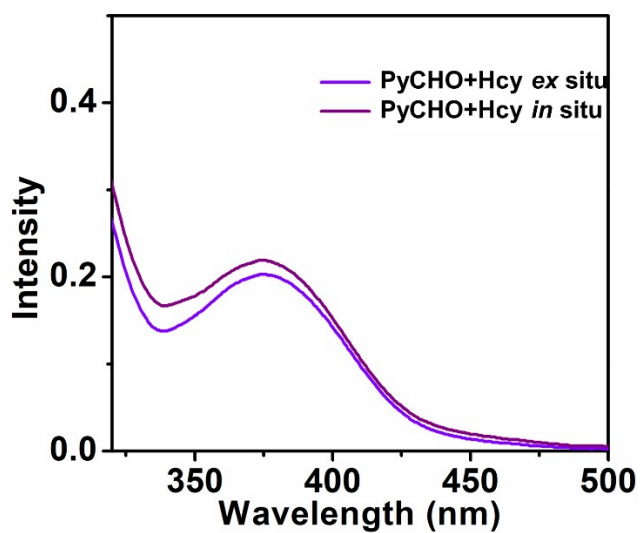


Figure S12. Absorption spectra of PyCHO+Hcy *in situ* and PyCHO+Hcy *ex situ*. PyCHO+Hcy *in situ* is the product prepared *in situ* by addition of 80 equiv. of Hcy to a solution of PyCHO; PyCHO+Hcy *ex situ* is the isolated product.

PyCHO PyCHO+Cys PyCHO+Hcy

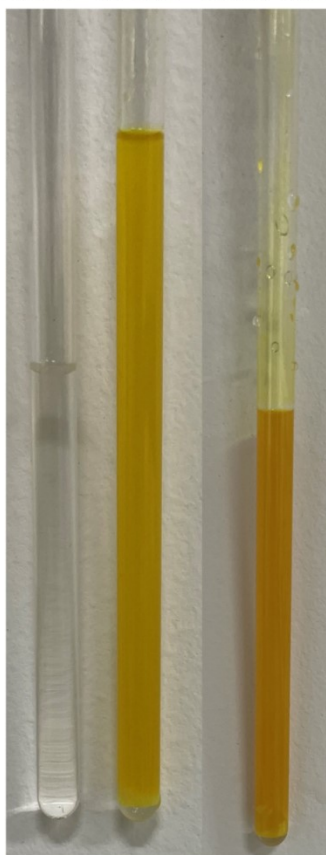


Figure S13. Color changes of **PyCHO** solution after addition of Cys and Hcy

Conductance measurements

Single-molecule conductance was measured using the Xtech STM break-junction under ambient conditions (room temperature 25°C), and the data is analyzed by XMe open-source code. More information is reported on previous papers¹⁻⁵. The STMBJ measurements were performed in TCB (1,2,4-trichlorobenzene, CNW Technologies) with a concentration of 0.1 mM. The samples (PyCHO+Cys / PyCHO+Hcy) for conductance measurement were prepared as follows: a solution of PyCHO (0.1 mM in TCB) was added 80 equiv. of Cys/Hcy. Then the mixture was sonicated for 30 min at ambient, and the supernatant was used for conductance measurement.

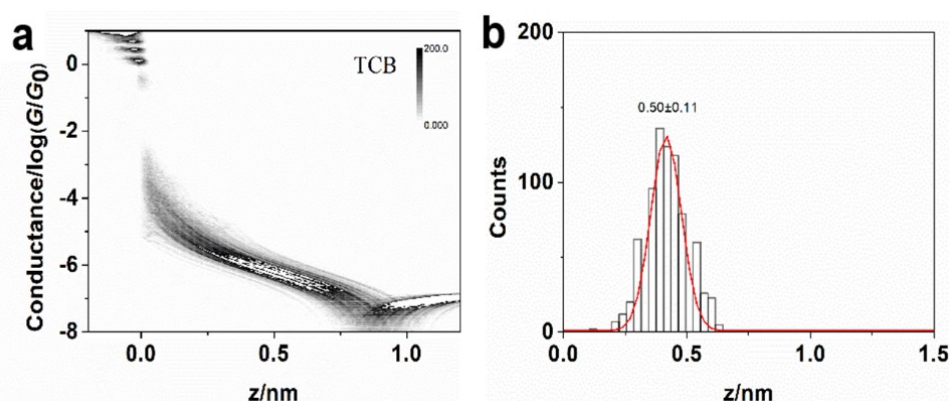


Figure S14. (a) Two-dimensional conductance histogram of blank solvent. (b) Relative displacement distribution. The conductance ranges to determine the relative displacement distribution are from $10^{-0.3}$ to $10^{-6.0} G_0$. No obvious conductance peak signal was found in the blank solvent measurement. The stretching distance is $\Delta z = 0.50 \pm 0.11$ nm (the error is the standard deviation), corresponding to the gold snap-back distance.

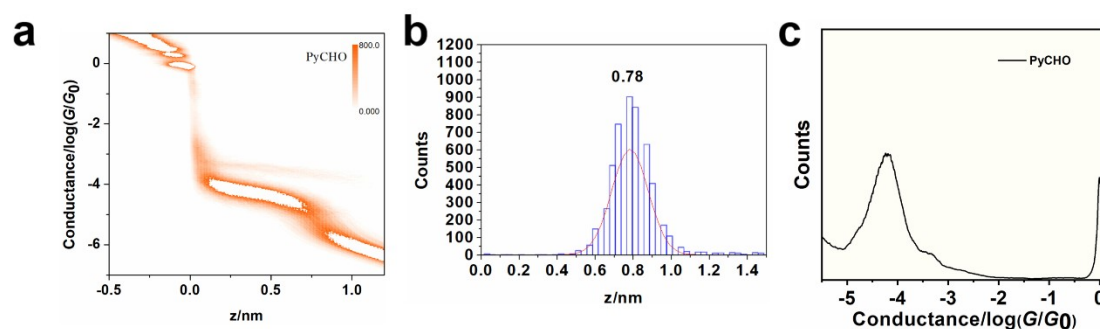


Figure S15. (a) 2D conductance histograms of PyCHO; (b) stretching distance histograms of PyCHO; (c) 1D conductance histograms of PyCHO.

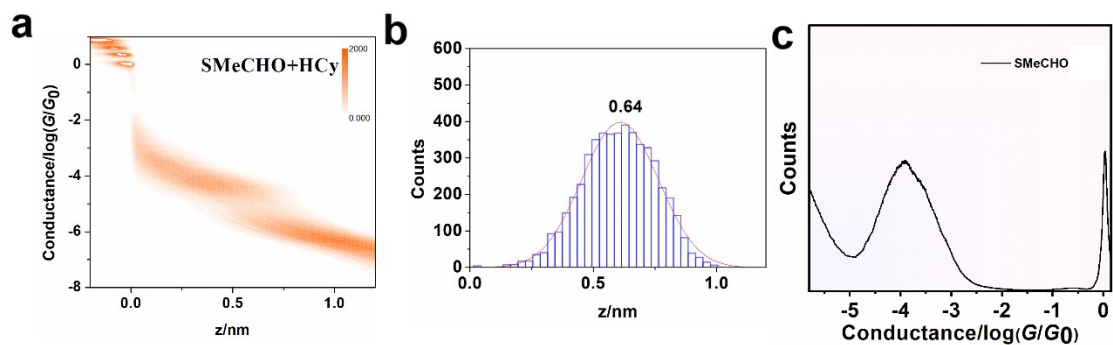


Figure S16. (a) 2D conductance histograms of SMeCHO; (b) stretching distance histograms of SMeCHO. (c) 1D conductance histograms of SMeCHO.

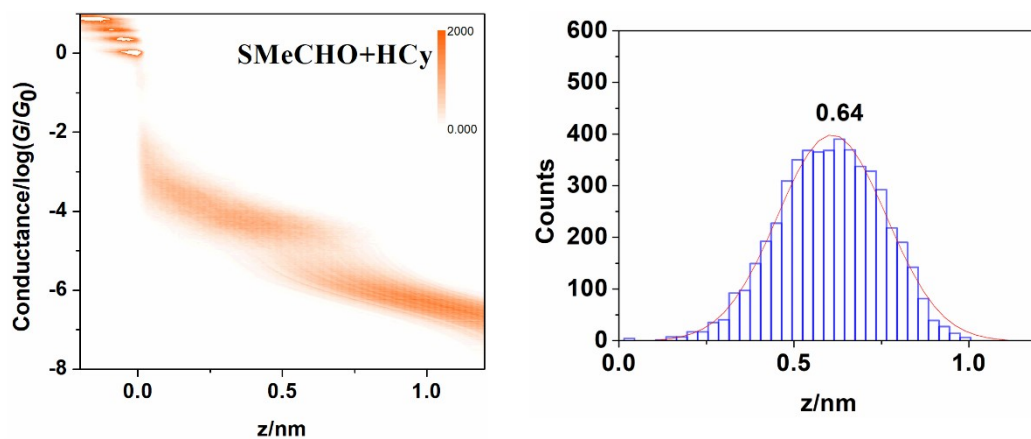


Figure S17. 2D conductance histograms of SMeCHO after reacting with Hcy (left); stretching distance histograms of SMeCHO+Hcy (right).

DFT Calculations

The geometry optimizations of the molecules were carried out using ω B97XD functional and 6-311G(d,p) basis set in Gaussian 09 package, and the frequency analysis was performed at the same theoretical level to verify that the stationary points are minimums or transition states. An electric field of 0.0514 V/nm was applied while optimizing the molecular structure and the direction of electrical field is along with the molecular backbone. Then, the optimized molecular structures were placed between two gold electrodes to construct the single-molecule junctions. The surface configuration of the gold electrode is constructed as a pyramid.^{6,7} In the initial configuration of the device, the distance between the N atom and the gold atom of the electrode was controlled at about 2.3 Å. In configuration optimization, the coordinates of all gold atoms in the electrode are fixed and there are no restrictions on the coordinates of the molecules. The geometry optimization and the transmission spectrum of single-molecule junction were performed using the Quantum ATKQ-2019.12 package.⁸ The FHI pseudopotential with a double- ζ basis set was used for Au atoms, and the PseudoDojo pseudopotential with a medium basis set was used for other atoms. A real-space grid with an equivalent energy cutoff of 80 Hartree and the k-points of 3, 3, 134 was used for geometry optimization, and the force threshold is 0.05 eV/Å. In the transmission calculation, transverse k points are increased to 7, 7. The Au–N is about 2.2 Å and coplanar with the pyridine ring in the initial configurations of the molecular junctions without Au– π interaction. When the gold atom and the pyridine ring are not coplanar, and the distance between the gold atom and the pyridine is close to about 2.2 Å, the orbital of the gold atom overlaps with the π -electron orbital of the pyridine ring, resulting in the Au– π interaction in the junctions.

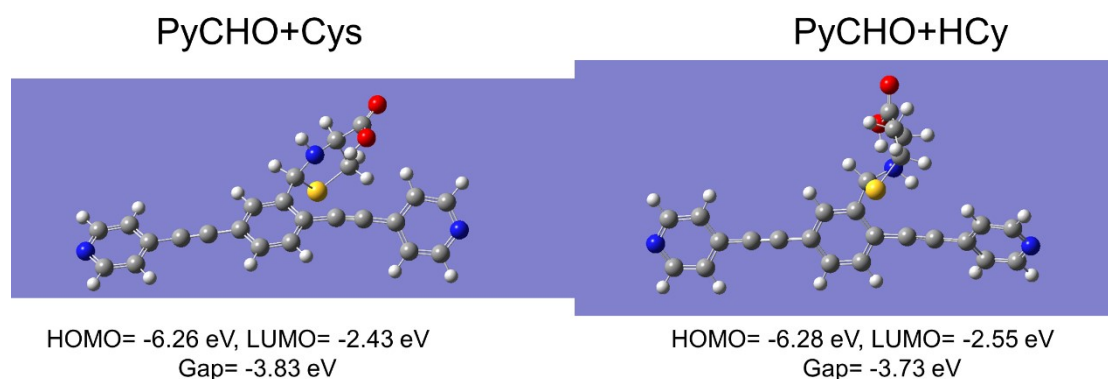


Figure S18. The optimal structures of PyCHO+Cys (left) and PyCHO+HCy (right).

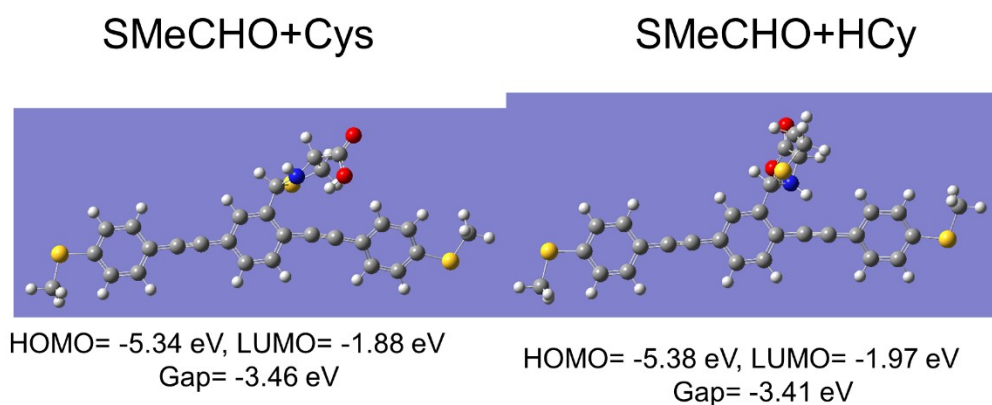


Figure S19. The optimal structures of SMeCHO+Cys (left) and SMeCHO+Hcy (right).

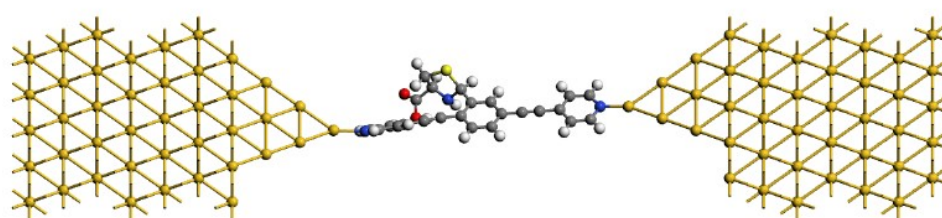


Figure S20. The geometries for PyCHO+Cys without Au- π interaction.

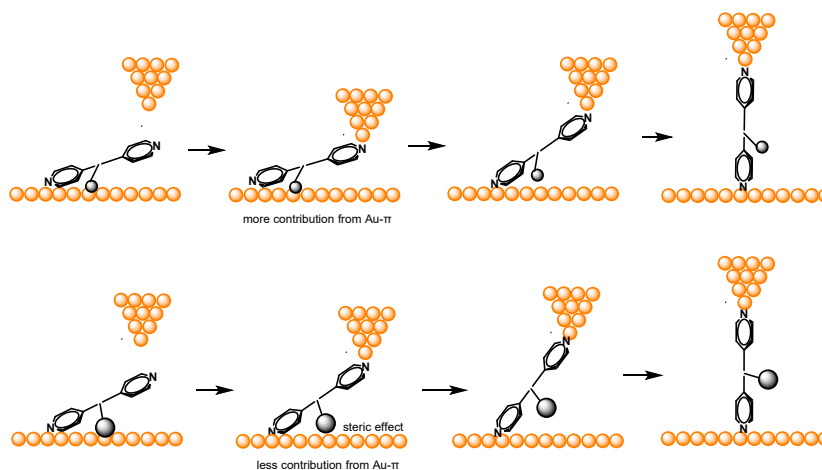


Figure S21. The influence of side rings on electrode-molecule interactions. Up, PyCHO+Hcy; down, PyCHO+Cys.

For PyCHO+Cys and PyCHO+Hcy, beside the pyridine anchors, the S and N atoms in the side chains can also bind with Au substrate, thus the binding structures above are the most favorable ones before the formation of junction.

The coordinates of calculated results of PyCHO+Cys

Item: 1

Location: cy3.hdf5

Name: DeviceConfiguration_0

Type: DeviceConfiguration

+-----+

| Central region Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

u_1 = 14.418791 0.000000 0.000000 Ang

u_2 = -7.209396 12.487039 0.000000 Ang

u_3 = 0.000000 0.000000 47.313141 Ang

+-----+

| Central region: Cartesian (Angstrom) / fractional |

+-----+

267

Central region

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | -7.078130e-03 | 3.961677e-02 | 1.177289e+00 | 0.00110 | 0.00317 | 0.02488 |
| Au | 1.434801e+00 | 8.720861e-01 | 3.531868e+00 | 0.13443 | 0.06984 | 0.07465 |
| Au | -7.078130e-03 | 1.704555e+00 | 5.886447e+00 | 0.06776 | 0.13651 | 0.12441 |
| Au | -1.448957e+00 | 2.537025e+00 | 1.177289e+00 | 0.00110 | 0.20317 | 0.02488 |
| Au | -7.078130e-03 | 3.369494e+00 | 3.531868e+00 | 0.13443 | 0.26984 | 0.07465 |
| Au | -1.448957e+00 | 4.201963e+00 | 5.886447e+00 | 0.06776 | 0.33651 | 0.12441 |
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| Au | -1.448957e+00 | 5.866902e+00 | 3.531868e+00 | 0.13443 | 0.46984 | 0.07465 |
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| Au | -4.332715e+00 | 7.531840e+00 | 1.177289e+00 | 0.00110 | 0.60317 | 0.02488 |
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| Au | -4.332715e+00 | 9.196779e+00 | 5.886447e+00 | 0.06776 | 0.73651 | 0.12441 |
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| Au | -5.774595e+00 | 1.169419e+01 | 5.886447e+00 | 0.06776 | 0.93651 | 0.12441 |
| Au | 2.876680e+00 | 3.961677e-02 | 1.177289e+00 | 0.20110 | 0.00317 | 0.02488 |
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| Au | 2.876680e+00 | 1.704555e+00 | 5.886447e+00 | 0.26776 | 0.13651 | 0.12441 |
| Au | 1.434801e+00 | 2.537025e+00 | 1.177289e+00 | 0.20110 | 0.20317 | 0.02488 |
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| Au | 1.008608e+01 | 2.537025e+00 | 1.177289e+00 | 0.80110 | 0.20317 | 0.02488 |

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|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 1.152795e+01 | 3.369494e+00 | 3.531868e+00 | 0.93443 | 0.26984 | 0.07465 |
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| Au | 8.644197e+00 | 5.034433e+00 | 1.177289e+00 | 0.80110 | 0.40317 | 0.02488 |
| Au | 1.008608e+01 | 5.866902e+00 | 3.531868e+00 | 0.93443 | 0.46984 | 0.07465 |
| Au | 8.644197e+00 | 6.699371e+00 | 5.886447e+00 | 0.86776 | 0.53651 | 0.12441 |
| Au | 7.202317e+00 | 7.531840e+00 | 1.177289e+00 | 0.80110 | 0.60317 | 0.02488 |
| Au | 8.644197e+00 | 8.364310e+00 | 3.531868e+00 | 0.93443 | 0.66984 | 0.07465 |
| Au | 7.202317e+00 | 9.196779e+00 | 5.886447e+00 | 0.86776 | 0.73651 | 0.12441 |
| Au | 5.760438e+00 | 1.002925e+01 | 1.177289e+00 | 0.80110 | 0.80317 | 0.02488 |
| Au | 7.202317e+00 | 1.086172e+01 | 3.531868e+00 | 0.93443 | 0.86984 | 0.07465 |
| Au | 5.760438e+00 | 1.169419e+01 | 5.886447e+00 | 0.86776 | 0.93651 | 0.12441 |
| Au | -7.078130e-03 | 3.961677e-02 | 8.241026e+00 | 0.00110 | 0.00317 | 0.17418 |
| Au | 5.760438e+00 | 3.961677e-02 | 8.241026e+00 | 0.40110 | 0.00317 | 0.17418 |
| Au | 8.644197e+00 | 3.961677e-02 | 8.241026e+00 | 0.60110 | 0.00317 | 0.17418 |
| Au | 1.152795e+01 | 3.961677e-02 | 8.241026e+00 | 0.80110 | 0.00317 | 0.17418 |
| Au | 2.876680e+00 | 3.961677e-02 | 8.241026e+00 | 0.20110 | 0.00317 | 0.17418 |
| Au | -1.448957e+00 | 2.537025e+00 | 8.241026e+00 | 0.00110 | 0.20317 | 0.17418 |
| Au | 1.434801e+00 | 2.537025e+00 | 8.241026e+00 | 0.20110 | 0.20317 | 0.17418 |
| Au | 4.318559e+00 | 2.537025e+00 | 8.241026e+00 | 0.40110 | 0.20317 | 0.17418 |
| Au | 7.202317e+00 | 2.537025e+00 | 8.241026e+00 | 0.60110 | 0.20317 | 0.17418 |
| Au | 1.008608e+01 | 2.537025e+00 | 8.241026e+00 | 0.80110 | 0.20317 | 0.17418 |
| Au | -2.890836e+00 | 5.034433e+00 | 8.241026e+00 | 0.00110 | 0.40317 | 0.17418 |
| Au | -7.078130e-03 | 5.034433e+00 | 8.241026e+00 | 0.20110 | 0.40317 | 0.17418 |
| Au | 2.876680e+00 | 5.034433e+00 | 8.241026e+00 | 0.40110 | 0.40317 | 0.17418 |
| Au | 5.760438e+00 | 5.034433e+00 | 8.241026e+00 | 0.60110 | 0.40317 | 0.17418 |
| Au | 8.644197e+00 | 5.034433e+00 | 8.241026e+00 | 0.80110 | 0.40317 | 0.17418 |
| Au | -4.332715e+00 | 7.531840e+00 | 8.241026e+00 | 0.00110 | 0.60317 | 0.17418 |
| Au | -1.448957e+00 | 7.531840e+00 | 8.241026e+00 | 0.20110 | 0.60317 | 0.17418 |
| Au | 1.434801e+00 | 7.531840e+00 | 8.241026e+00 | 0.40110 | 0.60317 | 0.17418 |
| Au | 4.318559e+00 | 7.531840e+00 | 8.241026e+00 | 0.60110 | 0.60317 | 0.17418 |
| Au | 7.202317e+00 | 7.531840e+00 | 8.241026e+00 | 0.80110 | 0.60317 | 0.17418 |
| Au | -5.774595e+00 | 1.002925e+01 | 8.241026e+00 | 0.00110 | 0.80317 | 0.17418 |
| Au | -2.890836e+00 | 1.002925e+01 | 8.241026e+00 | 0.20110 | 0.80317 | 0.17418 |
| Au | -7.078130e-03 | 1.002925e+01 | 8.241026e+00 | 0.40110 | 0.80317 | 0.17418 |
| Au | 2.876680e+00 | 1.002925e+01 | 8.241026e+00 | 0.60110 | 0.80317 | 0.17418 |
| Au | 5.760438e+00 | 1.002925e+01 | 8.241026e+00 | 0.80110 | 0.80317 | 0.17418 |
| Au | -1.448957e+00 | 5.866902e+00 | 1.059560e+01 | 0.13443 | 0.46984 | 0.22395 |
| Au | 1.434801e+00 | 5.866902e+00 | 1.059560e+01 | 0.33443 | 0.46984 | 0.22395 |
| Au | 4.318559e+00 | 5.866902e+00 | 1.059560e+01 | 0.53443 | 0.46984 | 0.22395 |
| Au | -7.078130e-03 | 8.364310e+00 | 1.059560e+01 | 0.33443 | 0.66984 | 0.22395 |
| Au | 2.876680e+00 | 8.364310e+00 | 1.059560e+01 | 0.53443 | 0.66984 | 0.22395 |
| Au | 1.434801e+00 | 1.086172e+01 | 1.059560e+01 | 0.53443 | 0.86984 | 0.22395 |
| Au | -7.078130e-03 | 6.699371e+00 | 1.295018e+01 | 0.26776 | 0.53651 | 0.27371 |
| Au | 2.876680e+00 | 6.699371e+00 | 1.295018e+01 | 0.46776 | 0.53651 | 0.27371 |

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| Au | 1.434801e+00 | 9.196779e+00 | 1.295018e+01 | 0.46776 | 0.73651 | 0.27371 |
| H | 4.661897e+00 | 4.696949e+00 | 1.340434e+01 | 0.51139 | 0.37615 | 0.28331 |
| N | 2.620843e+00 | 4.697288e+00 | 1.382321e+01 | 0.36985 | 0.37617 | 0.29216 |
| C | 3.911989e+00 | 4.880893e+00 | 1.418820e+01 | 0.46675 | 0.39088 | 0.29988 |
| H | 6.078030e-01 | 4.799230e+00 | 1.436519e+01 | 0.23432 | 0.38434 | 0.30362 |
| C | 1.639142e+00 | 4.927710e+00 | 1.472396e+01 | 0.31099 | 0.39463 | 0.31120 |
| Au | 1.434801e+00 | 7.531840e+00 | 1.530476e+01 | 0.40110 | 0.60317 | 0.32348 |
| C | 4.280951e+00 | 5.251228e+00 | 1.547040e+01 | 0.50717 | 0.42053 | 0.32698 |
| H | 5.342208e+00 | 5.323498e+00 | 1.573845e+01 | 0.58366 | 0.42632 | 0.33264 |
| C | 1.909645e+00 | 5.287619e+00 | 1.603577e+01 | 0.34417 | 0.42345 | 0.33893 |
| C | 3.265928e+00 | 5.423691e+00 | 1.644997e+01 | 0.44368 | 0.43435 | 0.34768 |
| H | 1.092641e+00 | 5.433390e+00 | 1.675591e+01 | 0.29334 | 0.43512 | 0.35415 |
| O | 8.457287e+00 | 5.318237e+00 | 1.677087e+01 | 0.79950 | 0.42590 | 0.35447 |
| O | 6.588224e+00 | 4.229607e+00 | 1.744911e+01 | 0.62628 | 0.33872 | 0.36880 |
| C | 7.604630e+00 | 5.109363e+00 | 1.760557e+01 | 0.73200 | 0.40917 | 0.37211 |
| C | 3.558192e+00 | 5.604704e+00 | 1.781490e+01 | 0.47120 | 0.44884 | 0.37653 |
| H | 5.943987e+00 | 7.030429e+00 | 1.790456e+01 | 0.69375 | 0.56302 | 0.37843 |
| H | 6.090806e+00 | 4.303353e+00 | 1.832121e+01 | 0.59473 | 0.34463 | 0.38723 |
| H | 7.399605e+00 | 8.001127e+00 | 1.836121e+01 | 0.83357 | 0.64075 | 0.38808 |
| C | 6.722722e+00 | 7.186434e+00 | 1.867844e+01 | 0.75400 | 0.57551 | 0.39478 |
| C | 7.501614e+00 | 5.882989e+00 | 1.893816e+01 | 0.75583 | 0.47113 | 0.40027 |
| C | 3.720216e+00 | 5.550469e+00 | 1.904212e+01 | 0.48026 | 0.44450 | 0.40247 |
| H | 8.528495e+00 | 6.105426e+00 | 1.930406e+01 | 0.83596 | 0.48894 | 0.40801 |
| N | 6.677660e+00 | 5.106714e+00 | 1.986871e+01 | 0.66760 | 0.40896 | 0.41994 |
| H | 1.578396e+00 | 4.581019e+00 | 2.010861e+01 | 0.29290 | 0.36686 | 0.42501 |
| S | 5.921038e+00 | 7.625613e+00 | 2.024749e+01 | 0.71599 | 0.61068 | 0.42795 |
| H | 7.224702e+00 | 4.353798e+00 | 2.030227e+01 | 0.67539 | 0.34867 | 0.42910 |
| C | 3.630334e+00 | 5.222300e+00 | 2.041000e+01 | 0.46089 | 0.41822 | 0.43138 |
| C | 2.386756e+00 | 4.680127e+00 | 2.084692e+01 | 0.35293 | 0.37480 | 0.44062 |
| C | 6.051165e+00 | 5.917764e+00 | 2.092697e+01 | 0.65663 | 0.47391 | 0.44231 |
| C | 4.711044e+00 | 5.348420e+00 | 2.133905e+01 | 0.54089 | 0.42832 | 0.45102 |
| H | 6.696266e+00 | 5.977497e+00 | 2.183350e+01 | 0.70376 | 0.47870 | 0.46147 |
| C | 2.202304e+00 | 4.271335e+00 | 2.215694e+01 | 0.32377 | 0.34206 | 0.46830 |
| H | 1.237739e+00 | 3.860004e+00 | 2.248593e+01 | 0.24040 | 0.30912 | 0.47526 |
| C | 4.517183e+00 | 4.932517e+00 | 2.264903e+01 | 0.51079 | 0.39501 | 0.47870 |
| C | 3.272380e+00 | 4.396146e+00 | 2.308600e+01 | 0.40298 | 0.35206 | 0.48794 |
| H | 5.335621e+00 | 5.016615e+00 | 2.338003e+01 | 0.57092 | 0.40175 | 0.49416 |
| C | 3.121866e+00 | 4.049844e+00 | 2.443765e+01 | 0.37868 | 0.32432 | 0.51651 |
| C | 3.037220e+00 | 3.826943e+00 | 2.565004e+01 | 0.36388 | 0.30647 | 0.54213 |
| C | 2.935504e+00 | 3.719666e+00 | 2.704408e+01 | 0.35253 | 0.29788 | 0.57160 |
| H | 9.062082e-01 | 2.890013e+00 | 2.706232e+01 | 0.17857 | 0.23144 | 0.57198 |
| H | 4.929533e+00 | 4.545081e+00 | 2.744742e+01 | 0.52387 | 0.36398 | 0.58012 |
| C | 1.755572e+00 | 3.228680e+00 | 2.766978e+01 | 0.25104 | 0.25856 | 0.58482 |
| C | 4.002586e+00 | 4.150602e+00 | 2.788420e+01 | 0.44379 | 0.33239 | 0.58935 |

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| C | 1.690108e+00 | 3.199377e+00 | 2.905260e+01 | 0.24532 | 0.25622 | 0.61405 |
| C | 3.844786e+00 | 4.087165e+00 | 2.925805e+01 | 0.43031 | 0.32731 | 0.61839 |
| H | 7.972210e-01 | 2.832817e+00 | 2.958055e+01 | 0.16872 | 0.22686 | 0.62521 |
| N | 2.710948e+00 | 3.622868e+00 | 2.983511e+01 | 0.33308 | 0.29013 | 0.63059 |
| H | 4.632821e+00 | 4.419077e+00 | 2.995045e+01 | 0.49825 | 0.35389 | 0.63303 |
| Au | 3.076680e+00 | 3.369494e+00 | 3.200838e+01 | 0.34830 | 0.26984 | 0.67652 |
| Au | 3.076680e+00 | 1.704555e+00 | 3.436296e+01 | 0.28163 | 0.13651 | 0.72629 |
| Au | 1.634801e+00 | 4.201963e+00 | 3.436296e+01 | 0.28163 | 0.33651 | 0.72629 |
| Au | 4.518559e+00 | 4.201963e+00 | 3.436296e+01 | 0.48163 | 0.33651 | 0.72629 |
| Au | 3.076680e+00 | 3.961677e-02 | 3.671754e+01 | 0.21497 | 0.00317 | 0.77605 |
| Au | 1.634801e+00 | 2.537025e+00 | 3.671754e+01 | 0.21497 | 0.20317 | 0.77605 |
| Au | 4.518559e+00 | 2.537025e+00 | 3.671754e+01 | 0.41497 | 0.20317 | 0.77605 |
| Au | 1.929219e-01 | 5.034433e+00 | 3.671754e+01 | 0.21497 | 0.40317 | 0.77605 |
| Au | 3.076680e+00 | 5.034433e+00 | 3.671754e+01 | 0.41497 | 0.40317 | 0.77605 |
| Au | 5.960438e+00 | 5.034433e+00 | 3.671754e+01 | 0.61497 | 0.40317 | 0.77605 |
| Au | 1.634801e+00 | 8.720861e-01 | 3.907212e+01 | 0.14830 | 0.06984 | 0.82582 |
| Au | 4.518559e+00 | 8.720861e-01 | 3.907212e+01 | 0.34830 | 0.06984 | 0.82582 |
| Au | 7.402317e+00 | 8.720861e-01 | 3.907212e+01 | 0.54830 | 0.06984 | 0.82582 |
| Au | 1.028608e+01 | 8.720861e-01 | 3.907212e+01 | 0.74830 | 0.06984 | 0.82582 |
| Au | 1.316983e+01 | 8.720861e-01 | 3.907212e+01 | 0.94830 | 0.06984 | 0.82582 |
| Au | 1.929219e-01 | 3.369494e+00 | 3.907212e+01 | 0.14830 | 0.26984 | 0.82582 |
| Au | 3.076680e+00 | 3.369494e+00 | 3.907212e+01 | 0.34830 | 0.26984 | 0.82582 |
| Au | 5.960438e+00 | 3.369494e+00 | 3.907212e+01 | 0.54830 | 0.26984 | 0.82582 |
| Au | 8.844197e+00 | 3.369494e+00 | 3.907212e+01 | 0.74830 | 0.26984 | 0.82582 |
| Au | 1.172795e+01 | 3.369494e+00 | 3.907212e+01 | 0.94830 | 0.26984 | 0.82582 |
| Au | -1.248957e+00 | 5.866902e+00 | 3.907212e+01 | 0.14830 | 0.46984 | 0.82582 |
| Au | 1.634801e+00 | 5.866902e+00 | 3.907212e+01 | 0.34830 | 0.46984 | 0.82582 |
| Au | 4.518559e+00 | 5.866902e+00 | 3.907212e+01 | 0.54830 | 0.46984 | 0.82582 |
| Au | 7.402317e+00 | 5.866902e+00 | 3.907212e+01 | 0.74830 | 0.46984 | 0.82582 |
| Au | 1.028608e+01 | 5.866902e+00 | 3.907212e+01 | 0.94830 | 0.46984 | 0.82582 |
| Au | -2.690836e+00 | 8.364310e+00 | 3.907212e+01 | 0.14830 | 0.66984 | 0.82582 |
| Au | 1.929219e-01 | 8.364310e+00 | 3.907212e+01 | 0.34830 | 0.66984 | 0.82582 |
| Au | 3.076680e+00 | 8.364310e+00 | 3.907212e+01 | 0.54830 | 0.66984 | 0.82582 |
| Au | 5.960438e+00 | 8.364310e+00 | 3.907212e+01 | 0.74830 | 0.66984 | 0.82582 |
| Au | 8.844197e+00 | 8.364310e+00 | 3.907212e+01 | 0.94830 | 0.66984 | 0.82582 |
| Au | -4.132715e+00 | 1.086172e+01 | 3.907212e+01 | 0.14830 | 0.86984 | 0.82582 |
| Au | -1.248957e+00 | 1.086172e+01 | 3.907212e+01 | 0.34830 | 0.86984 | 0.82582 |
| Au | 1.634801e+00 | 1.086172e+01 | 3.907212e+01 | 0.54830 | 0.86984 | 0.82582 |
| Au | 4.518559e+00 | 1.086172e+01 | 3.907212e+01 | 0.74830 | 0.86984 | 0.82582 |
| Au | 7.402317e+00 | 1.086172e+01 | 3.907212e+01 | 0.94830 | 0.86984 | 0.82582 |
| Au | 1.929219e-01 | 1.704555e+00 | 4.142669e+01 | 0.08163 | 0.13651 | 0.87559 |
| Au | 1.929219e-01 | 3.961677e-02 | 4.378127e+01 | 0.01497 | 0.00317 | 0.92535 |
| Au | 1.634801e+00 | 8.720861e-01 | 4.613585e+01 | 0.14830 | 0.06984 | 0.97512 |
| Au | -1.248957e+00 | 4.201963e+00 | 4.142669e+01 | 0.08163 | 0.33651 | 0.87559 |

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| Au | -1.248957e+00 | 2.537025e+00 | 4.378127e+01 | 0.01497 | 0.20317 | 0.92535 |
| Au | 1.929219e-01 | 3.369494e+00 | 4.613585e+01 | 0.14830 | 0.26984 | 0.97512 |
| Au | -2.690836e+00 | 6.699371e+00 | 4.142669e+01 | 0.08163 | 0.53651 | 0.87559 |
| Au | -2.690836e+00 | 5.034433e+00 | 4.378127e+01 | 0.01497 | 0.40317 | 0.92535 |
| Au | -1.248957e+00 | 5.866902e+00 | 4.613585e+01 | 0.14830 | 0.46984 | 0.97512 |
| Au | -4.132715e+00 | 9.196779e+00 | 4.142669e+01 | 0.08163 | 0.73651 | 0.87559 |
| Au | -4.132715e+00 | 7.531840e+00 | 4.378127e+01 | 0.01497 | 0.60317 | 0.92535 |
| Au | -2.690836e+00 | 8.364310e+00 | 4.613585e+01 | 0.14830 | 0.66984 | 0.97512 |
| Au | -5.574595e+00 | 1.169419e+01 | 4.142669e+01 | 0.08163 | 0.93651 | 0.87559 |
| Au | -5.574595e+00 | 1.002925e+01 | 4.378127e+01 | 0.01497 | 0.80317 | 0.92535 |
| Au | -4.132715e+00 | 1.086172e+01 | 4.613585e+01 | 0.14830 | 0.86984 | 0.97512 |
| Au | 3.076680e+00 | 1.704555e+00 | 4.142669e+01 | 0.28163 | 0.13651 | 0.87559 |
| Au | 3.076680e+00 | 3.961677e-02 | 4.378127e+01 | 0.21497 | 0.00317 | 0.92535 |
| Au | 4.518559e+00 | 8.720861e-01 | 4.613585e+01 | 0.34830 | 0.06984 | 0.97512 |
| Au | 1.634801e+00 | 4.201963e+00 | 4.142669e+01 | 0.28163 | 0.33651 | 0.87559 |
| Au | 1.634801e+00 | 2.537025e+00 | 4.378127e+01 | 0.21497 | 0.20317 | 0.92535 |
| Au | 3.076680e+00 | 3.369494e+00 | 4.613585e+01 | 0.34830 | 0.26984 | 0.97512 |
| Au | 1.929219e-01 | 6.699371e+00 | 4.142669e+01 | 0.28163 | 0.53651 | 0.87559 |
| Au | 1.929219e-01 | 5.034433e+00 | 4.378127e+01 | 0.21497 | 0.40317 | 0.92535 |
| Au | 1.634801e+00 | 5.866902e+00 | 4.613585e+01 | 0.34830 | 0.46984 | 0.97512 |
| Au | -1.248957e+00 | 9.196779e+00 | 4.142669e+01 | 0.28163 | 0.73651 | 0.87559 |
| Au | -1.248957e+00 | 7.531840e+00 | 4.378127e+01 | 0.21497 | 0.60317 | 0.92535 |
| Au | 1.929219e-01 | 8.364310e+00 | 4.613585e+01 | 0.34830 | 0.66984 | 0.97512 |
| Au | -2.690836e+00 | 1.169419e+01 | 4.142669e+01 | 0.28163 | 0.93651 | 0.87559 |
| Au | -2.690836e+00 | 1.002925e+01 | 4.378127e+01 | 0.21497 | 0.80317 | 0.92535 |
| Au | -1.248957e+00 | 1.086172e+01 | 4.613585e+01 | 0.34830 | 0.86984 | 0.97512 |
| Au | 5.960438e+00 | 1.704555e+00 | 4.142669e+01 | 0.48163 | 0.13651 | 0.87559 |
| Au | 5.960438e+00 | 3.961677e-02 | 4.378127e+01 | 0.41497 | 0.00317 | 0.92535 |
| Au | 7.402317e+00 | 8.720861e-01 | 4.613585e+01 | 0.54830 | 0.06984 | 0.97512 |
| Au | 4.518559e+00 | 4.201963e+00 | 4.142669e+01 | 0.48163 | 0.33651 | 0.87559 |
| Au | 4.518559e+00 | 2.537025e+00 | 4.378127e+01 | 0.41497 | 0.20317 | 0.92535 |
| Au | 5.960438e+00 | 3.369494e+00 | 4.613585e+01 | 0.54830 | 0.26984 | 0.97512 |
| Au | 3.076680e+00 | 6.699371e+00 | 4.142669e+01 | 0.48163 | 0.53651 | 0.87559 |
| Au | 3.076680e+00 | 5.034433e+00 | 4.378127e+01 | 0.41497 | 0.40317 | 0.92535 |
| Au | 4.518559e+00 | 5.866902e+00 | 4.613585e+01 | 0.54830 | 0.46984 | 0.97512 |
| Au | 1.634801e+00 | 9.196779e+00 | 4.142669e+01 | 0.48163 | 0.73651 | 0.87559 |
| Au | 1.634801e+00 | 7.531840e+00 | 4.378127e+01 | 0.41497 | 0.60317 | 0.92535 |
| Au | 3.076680e+00 | 8.364310e+00 | 4.613585e+01 | 0.54830 | 0.66984 | 0.97512 |
| Au | 1.929219e-01 | 1.169419e+01 | 4.142669e+01 | 0.48163 | 0.93651 | 0.87559 |
| Au | 1.929219e-01 | 1.002925e+01 | 4.378127e+01 | 0.41497 | 0.80317 | 0.92535 |
| Au | 1.634801e+00 | 1.086172e+01 | 4.613585e+01 | 0.54830 | 0.86984 | 0.97512 |
| Au | 8.844197e+00 | 1.704555e+00 | 4.142669e+01 | 0.68163 | 0.13651 | 0.87559 |
| Au | 8.844197e+00 | 3.961677e-02 | 4.378127e+01 | 0.61497 | 0.00317 | 0.92535 |
| Au | 1.028608e+01 | 8.720861e-01 | 4.613585e+01 | 0.74830 | 0.06984 | 0.97512 |

| | | | | | | |
|----|--------------|--------------|--------------|---------|---------|---------|
| Au | 7.402317e+00 | 4.201963e+00 | 4.142669e+01 | 0.68163 | 0.33651 | 0.87559 |
| Au | 7.402317e+00 | 2.537025e+00 | 4.378127e+01 | 0.61497 | 0.20317 | 0.92535 |
| Au | 8.844197e+00 | 3.369494e+00 | 4.613585e+01 | 0.74830 | 0.26984 | 0.97512 |
| Au | 5.960438e+00 | 6.699371e+00 | 4.142669e+01 | 0.68163 | 0.53651 | 0.87559 |
| Au | 5.960438e+00 | 5.034433e+00 | 4.378127e+01 | 0.61497 | 0.40317 | 0.92535 |
| Au | 7.402317e+00 | 5.866902e+00 | 4.613585e+01 | 0.74830 | 0.46984 | 0.97512 |
| Au | 4.518559e+00 | 9.196779e+00 | 4.142669e+01 | 0.68163 | 0.73651 | 0.87559 |
| Au | 4.518559e+00 | 7.531840e+00 | 4.378127e+01 | 0.61497 | 0.60317 | 0.92535 |
| Au | 5.960438e+00 | 8.364310e+00 | 4.613585e+01 | 0.74830 | 0.66984 | 0.97512 |
| Au | 3.076680e+00 | 1.169419e+01 | 4.142669e+01 | 0.68163 | 0.93651 | 0.87559 |
| Au | 3.076680e+00 | 1.002925e+01 | 4.378127e+01 | 0.61497 | 0.80317 | 0.92535 |
| Au | 4.518559e+00 | 1.086172e+01 | 4.613585e+01 | 0.74830 | 0.86984 | 0.97512 |
| Au | 1.172795e+01 | 1.704555e+00 | 4.142669e+01 | 0.88163 | 0.13651 | 0.87559 |
| Au | 1.172795e+01 | 3.961677e-02 | 4.378127e+01 | 0.81497 | 0.00317 | 0.92535 |
| Au | 1.316983e+01 | 8.720861e-01 | 4.613585e+01 | 0.94830 | 0.06984 | 0.97512 |
| Au | 1.028608e+01 | 4.201963e+00 | 4.142669e+01 | 0.88163 | 0.33651 | 0.87559 |
| Au | 1.028608e+01 | 2.537025e+00 | 4.378127e+01 | 0.81497 | 0.20317 | 0.92535 |
| Au | 1.172795e+01 | 3.369494e+00 | 4.613585e+01 | 0.94830 | 0.26984 | 0.97512 |
| Au | 8.844197e+00 | 6.699371e+00 | 4.142669e+01 | 0.88163 | 0.53651 | 0.87559 |
| Au | 8.844197e+00 | 5.034433e+00 | 4.378127e+01 | 0.81497 | 0.40317 | 0.92535 |
| Au | 1.028608e+01 | 5.866902e+00 | 4.613585e+01 | 0.94830 | 0.46984 | 0.97512 |
| Au | 7.402317e+00 | 9.196779e+00 | 4.142669e+01 | 0.88163 | 0.73651 | 0.87559 |
| Au | 7.402317e+00 | 7.531840e+00 | 4.378127e+01 | 0.81497 | 0.60317 | 0.92535 |
| Au | 8.844197e+00 | 8.364310e+00 | 4.613585e+01 | 0.94830 | 0.66984 | 0.97512 |
| Au | 5.960438e+00 | 1.169419e+01 | 4.142669e+01 | 0.88163 | 0.93651 | 0.87559 |
| Au | 5.960438e+00 | 1.002925e+01 | 4.378127e+01 | 0.81497 | 0.80317 | 0.92535 |
| Au | 7.402317e+00 | 1.086172e+01 | 4.613585e+01 | 0.94830 | 0.86984 | 0.97512 |

+-----+

| Left electrode Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

u_1 = 2.883758 0.000000 0.000000 Ang

u_2 = -1.441879 2.497408 0.000000 Ang

u_3 = 0.000000 0.000000 7.063736 Ang

+-----+

| Left electrode: Cartesian (Angstrom) / fractional |

+-----+

3

Left electrode

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | -7.078130e-03 | 3.961677e-02 | 1.177289e+00 | 0.00548 | 0.01586 | 0.16667 |
| Au | 1.434801e+00 | 8.720861e-01 | 3.531868e+00 | 0.67214 | 0.34920 | 0.50000 |
| Au | -7.078130e-03 | 1.704555e+00 | 5.886447e+00 | 0.33881 | 0.68253 | 0.83333 |

+-----+

| Right electrode Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

| | | | |
|-------|-----------|----------|--------------|
| u_1 = | 2.883758 | 0.000000 | 0.000000 Ang |
| u_2 = | -1.441879 | 2.497408 | 0.000000 Ang |
| u_3 = | 0.000000 | 0.000000 | 7.063736 Ang |

+-----+

| Right electrode: Cartesian (Angstrom) / fractional |

+-----+

3

Right electrode

| | | | | | | |
|----|--------------|--------------|--------------|---------|---------|---------|
| Au | 1.929219e-01 | 1.704555e+00 | 1.177289e+00 | 0.40816 | 0.68253 | 0.16667 |
| Au | 1.929219e-01 | 3.961677e-02 | 3.531868e+00 | 0.07483 | 0.01586 | 0.50000 |
| Au | 1.634801e+00 | 8.720861e-01 | 5.886447e+00 | 0.74150 | 0.34920 | 0.83333 |

The coordinates of calculated results of PyCHO+Hcy

Item: 1

Location: hcys.hdf5

Name: DeviceConfiguration_0

Type: DeviceConfiguration

+-----+

| Central region Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

u_1 = 14.418791 0.000000 0.000000 Ang

u_2 = -7.209396 12.487039 0.000000 Ang

u_3 = 0.000000 0.000000 46.589136 Ang

+-----+

| Central region: Cartesian (Angstrom) / fractional |

+-----+

214

Central region

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 0.000000e+00 | 1.248704e+00 | 1.177289e+00 | 0.05000 | 0.10000 | 0.02527 |
| Au | 2.883758e+00 | 1.248704e+00 | 1.177289e+00 | 0.25000 | 0.10000 | 0.02527 |
| Au | 5.767516e+00 | 1.248704e+00 | 1.177289e+00 | 0.45000 | 0.10000 | 0.02527 |
| Au | 8.651275e+00 | 1.248704e+00 | 1.177289e+00 | 0.65000 | 0.10000 | 0.02527 |
| Au | 1.153503e+01 | 1.248704e+00 | 1.177289e+00 | 0.85000 | 0.10000 | 0.02527 |
| Au | -1.441879e+00 | 3.746112e+00 | 1.177289e+00 | 0.05000 | 0.30000 | 0.02527 |
| Au | 1.441879e+00 | 3.746112e+00 | 1.177289e+00 | 0.25000 | 0.30000 | 0.02527 |
| Au | 4.325637e+00 | 3.746112e+00 | 1.177289e+00 | 0.45000 | 0.30000 | 0.02527 |
| Au | 7.209396e+00 | 3.746112e+00 | 1.177289e+00 | 0.65000 | 0.30000 | 0.02527 |
| Au | 1.009315e+01 | 3.746112e+00 | 1.177289e+00 | 0.85000 | 0.30000 | 0.02527 |
| Au | -2.883758e+00 | 6.243520e+00 | 1.177289e+00 | 0.05000 | 0.50000 | 0.02527 |
| Au | -0.000000e+00 | 6.243520e+00 | 1.177289e+00 | 0.25000 | 0.50000 | 0.02527 |
| Au | 2.883758e+00 | 6.243520e+00 | 1.177289e+00 | 0.45000 | 0.50000 | 0.02527 |
| Au | 5.767516e+00 | 6.243520e+00 | 1.177289e+00 | 0.65000 | 0.50000 | 0.02527 |
| Au | 8.651275e+00 | 6.243520e+00 | 1.177289e+00 | 0.85000 | 0.50000 | 0.02527 |
| Au | -4.325637e+00 | 8.740928e+00 | 1.177289e+00 | 0.05000 | 0.70000 | 0.02527 |
| Au | -1.441879e+00 | 8.740928e+00 | 1.177289e+00 | 0.25000 | 0.70000 | 0.02527 |
| Au | 1.441879e+00 | 8.740928e+00 | 1.177289e+00 | 0.45000 | 0.70000 | 0.02527 |
| Au | 4.325637e+00 | 8.740928e+00 | 1.177289e+00 | 0.65000 | 0.70000 | 0.02527 |
| Au | 7.209396e+00 | 8.740928e+00 | 1.177289e+00 | 0.85000 | 0.70000 | 0.02527 |
| Au | -5.767516e+00 | 1.123834e+01 | 1.177289e+00 | 0.05000 | 0.90000 | 0.02527 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | -2.883758e+00 | 1.123834e+01 | 1.177289e+00 | 0.25000 | 0.90000 | 0.02527 |
| Au | -0.000000e+00 | 1.123834e+01 | 1.177289e+00 | 0.45000 | 0.90000 | 0.02527 |
| Au | 2.883758e+00 | 1.123834e+01 | 1.177289e+00 | 0.65000 | 0.90000 | 0.02527 |
| Au | 5.767516e+00 | 1.123834e+01 | 1.177289e+00 | 0.85000 | 0.90000 | 0.02527 |
| Au | 1.441879e+00 | 2.081173e+00 | 3.531868e+00 | 0.18333 | 0.16667 | 0.07581 |
| Au | 4.325637e+00 | 2.081173e+00 | 3.531868e+00 | 0.38333 | 0.16667 | 0.07581 |
| Au | 7.209396e+00 | 2.081173e+00 | 3.531868e+00 | 0.58333 | 0.16667 | 0.07581 |
| Au | 1.009315e+01 | 2.081173e+00 | 3.531868e+00 | 0.78333 | 0.16667 | 0.07581 |
| Au | 1.297691e+01 | 2.081173e+00 | 3.531868e+00 | 0.98333 | 0.16667 | 0.07581 |
| Au | -0.000000e+00 | 4.578581e+00 | 3.531868e+00 | 0.18333 | 0.36667 | 0.07581 |
| Au | 2.883758e+00 | 4.578581e+00 | 3.531868e+00 | 0.38333 | 0.36667 | 0.07581 |
| Au | 5.767516e+00 | 4.578581e+00 | 3.531868e+00 | 0.58333 | 0.36667 | 0.07581 |
| Au | 8.651275e+00 | 4.578581e+00 | 3.531868e+00 | 0.78333 | 0.36667 | 0.07581 |
| Au | 1.153503e+01 | 4.578581e+00 | 3.531868e+00 | 0.98333 | 0.36667 | 0.07581 |
| Au | -1.441879e+00 | 7.075989e+00 | 3.531868e+00 | 0.18333 | 0.56667 | 0.07581 |
| Au | 1.441879e+00 | 7.075989e+00 | 3.531868e+00 | 0.38333 | 0.56667 | 0.07581 |
| Au | 4.325637e+00 | 7.075989e+00 | 3.531868e+00 | 0.58333 | 0.56667 | 0.07581 |
| Au | 7.209396e+00 | 7.075989e+00 | 3.531868e+00 | 0.78333 | 0.56667 | 0.07581 |
| Au | 1.009315e+01 | 7.075989e+00 | 3.531868e+00 | 0.98333 | 0.56667 | 0.07581 |
| Au | -2.883758e+00 | 9.573397e+00 | 3.531868e+00 | 0.18333 | 0.76667 | 0.07581 |
| Au | -0.000000e+00 | 9.573397e+00 | 3.531868e+00 | 0.38333 | 0.76667 | 0.07581 |
| Au | 2.883758e+00 | 9.573397e+00 | 3.531868e+00 | 0.58333 | 0.76667 | 0.07581 |
| Au | 5.767516e+00 | 9.573397e+00 | 3.531868e+00 | 0.78333 | 0.76667 | 0.07581 |
| Au | 8.651275e+00 | 9.573397e+00 | 3.531868e+00 | 0.98333 | 0.76667 | 0.07581 |
| Au | -4.325637e+00 | 1.207080e+01 | 3.531868e+00 | 0.18333 | 0.96667 | 0.07581 |
| Au | -1.441879e+00 | 1.207080e+01 | 3.531868e+00 | 0.38333 | 0.96667 | 0.07581 |
| Au | 1.441879e+00 | 1.207080e+01 | 3.531868e+00 | 0.58333 | 0.96667 | 0.07581 |
| Au | 4.325637e+00 | 1.207080e+01 | 3.531868e+00 | 0.78333 | 0.96667 | 0.07581 |
| Au | 7.209396e+00 | 1.207080e+01 | 3.531868e+00 | 0.98333 | 0.96667 | 0.07581 |
| Au | 1.441879e+00 | 4.162346e-01 | 5.886447e+00 | 0.11667 | 0.03333 | 0.12635 |
| Au | 4.325637e+00 | 4.162346e-01 | 5.886447e+00 | 0.31667 | 0.03333 | 0.12635 |
| Au | 7.209396e+00 | 4.162346e-01 | 5.886447e+00 | 0.51667 | 0.03333 | 0.12635 |
| Au | 1.009315e+01 | 4.162346e-01 | 5.886447e+00 | 0.71667 | 0.03333 | 0.12635 |
| Au | 1.297691e+01 | 4.162346e-01 | 5.886447e+00 | 0.91667 | 0.03333 | 0.12635 |
| Au | -0.000000e+00 | 2.913643e+00 | 5.886447e+00 | 0.11667 | 0.23333 | 0.12635 |
| Au | 2.883758e+00 | 2.913643e+00 | 5.886447e+00 | 0.31667 | 0.23333 | 0.12635 |
| Au | 5.767516e+00 | 2.913643e+00 | 5.886447e+00 | 0.51667 | 0.23333 | 0.12635 |
| Au | 8.651275e+00 | 2.913643e+00 | 5.886447e+00 | 0.71667 | 0.23333 | 0.12635 |
| Au | 1.153503e+01 | 2.913643e+00 | 5.886447e+00 | 0.91667 | 0.23333 | 0.12635 |
| Au | -1.441879e+00 | 5.411050e+00 | 5.886447e+00 | 0.11667 | 0.43333 | 0.12635 |
| Au | 1.441879e+00 | 5.411050e+00 | 5.886447e+00 | 0.31667 | 0.43333 | 0.12635 |
| Au | 4.325637e+00 | 5.411050e+00 | 5.886447e+00 | 0.51667 | 0.43333 | 0.12635 |
| Au | 7.209396e+00 | 5.411050e+00 | 5.886447e+00 | 0.71667 | 0.43333 | 0.12635 |
| Au | 1.009315e+01 | 5.411050e+00 | 5.886447e+00 | 0.91667 | 0.43333 | 0.12635 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | -2.883758e+00 | 7.908458e+00 | 5.886447e+00 | 0.11667 | 0.63333 | 0.12635 |
| Au | -0.000000e+00 | 7.908458e+00 | 5.886447e+00 | 0.31667 | 0.63333 | 0.12635 |
| Au | 2.883758e+00 | 7.908458e+00 | 5.886447e+00 | 0.51667 | 0.63333 | 0.12635 |
| Au | 5.767516e+00 | 7.908458e+00 | 5.886447e+00 | 0.71667 | 0.63333 | 0.12635 |
| Au | 8.651275e+00 | 7.908458e+00 | 5.886447e+00 | 0.91667 | 0.63333 | 0.12635 |
| Au | -4.325637e+00 | 1.040587e+01 | 5.886447e+00 | 0.11667 | 0.83333 | 0.12635 |
| Au | -1.441879e+00 | 1.040587e+01 | 5.886447e+00 | 0.31667 | 0.83333 | 0.12635 |
| Au | 1.441879e+00 | 1.040587e+01 | 5.886447e+00 | 0.51667 | 0.83333 | 0.12635 |
| Au | 4.325637e+00 | 1.040587e+01 | 5.886447e+00 | 0.71667 | 0.83333 | 0.12635 |
| Au | 7.209396e+00 | 1.040587e+01 | 5.886447e+00 | 0.91667 | 0.83333 | 0.12635 |
| Au | 0.000000e+00 | 1.248704e+00 | 8.241026e+00 | 0.05000 | 0.10000 | 0.17689 |
| Au | 2.883758e+00 | 1.248704e+00 | 8.241026e+00 | 0.25000 | 0.10000 | 0.17689 |
| Au | 5.767516e+00 | 1.248704e+00 | 8.241026e+00 | 0.45000 | 0.10000 | 0.17689 |
| Au | 1.441879e+00 | 3.746112e+00 | 8.241026e+00 | 0.25000 | 0.30000 | 0.17689 |
| Au | 4.325637e+00 | 3.746112e+00 | 8.241026e+00 | 0.45000 | 0.30000 | 0.17689 |
| Au | 2.883758e+00 | 6.243520e+00 | 8.241026e+00 | 0.45000 | 0.50000 | 0.17689 |
| Au | 1.441879e+00 | 2.081173e+00 | 1.059560e+01 | 0.18333 | 0.16667 | 0.22743 |
| Au | 4.325637e+00 | 2.081173e+00 | 1.059560e+01 | 0.38333 | 0.16667 | 0.22743 |
| Au | 2.883758e+00 | 4.578581e+00 | 1.059560e+01 | 0.38333 | 0.36667 | 0.22743 |
| Au | 2.883758e+00 | 2.913643e+00 | 1.295018e+01 | 0.31667 | 0.23333 | 0.27797 |
| N | 2.916648e+00 | 3.069855e+00 | 1.507735e+01 | 0.32520 | 0.24584 | 0.32362 |
| H | 4.993903e+00 | 3.172893e+00 | 1.512136e+01 | 0.47339 | 0.25409 | 0.32457 |
| H | 8.410937e-01 | 2.987387e+00 | 1.518249e+01 | 0.17795 | 0.23924 | 0.32588 |
| C | 4.087383e+00 | 3.225361e+00 | 1.574137e+01 | 0.41262 | 0.25830 | 0.33788 |
| C | 1.757866e+00 | 3.112611e+00 | 1.577599e+01 | 0.24655 | 0.24927 | 0.33862 |
| C | 4.147458e+00 | 3.431370e+00 | 1.711130e+01 | 0.42504 | 0.27479 | 0.36728 |
| C | 1.716215e+00 | 3.306901e+00 | 1.714834e+01 | 0.25144 | 0.26483 | 0.36808 |
| H | 5.112271e+00 | 3.528856e+00 | 1.762792e+01 | 0.49586 | 0.28260 | 0.37837 |
| H | 7.540245e-01 | 3.328217e+00 | 1.767710e+01 | 0.18556 | 0.26653 | 0.37943 |
| C | 2.936422e+00 | 3.484320e+00 | 1.785982e+01 | 0.34317 | 0.27903 | 0.38335 |
| H | 7.151200e+00 | 4.537215e+00 | 1.907424e+01 | 0.67764 | 0.36335 | 0.40941 |
| C | 2.956234e+00 | 3.696298e+00 | 1.924995e+01 | 0.35303 | 0.29601 | 0.41319 |
| H | 6.078967e+00 | 6.948979e+00 | 1.942521e+01 | 0.69985 | 0.55650 | 0.41695 |
| H | 8.352402e+00 | 6.541067e+00 | 2.005657e+01 | 0.84119 | 0.52383 | 0.43050 |
| H | 4.465011e+00 | 5.725253e+00 | 2.031833e+01 | 0.53891 | 0.45850 | 0.43612 |
| C | 7.458218e+00 | 4.546056e+00 | 2.014181e+01 | 0.69929 | 0.36406 | 0.43233 |
| H | 8.434064e+00 | 4.027721e+00 | 2.021328e+01 | 0.74621 | 0.32255 | 0.43386 |
| C | 3.052981e+00 | 3.846070e+00 | 2.047557e+01 | 0.36574 | 0.30800 | 0.43949 |
| C | 6.269260e+00 | 6.761303e+00 | 2.050265e+01 | 0.70553 | 0.54147 | 0.44007 |
| C | 7.587148e+00 | 5.984760e+00 | 2.063218e+01 | 0.76584 | 0.47928 | 0.44285 |
| N | 5.080002e+00 | 6.081708e+00 | 2.106238e+01 | 0.59584 | 0.48704 | 0.45209 |
| O | 7.386652e+00 | 8.861461e+00 | 2.098433e+01 | 0.86712 | 0.70965 | 0.45041 |
| C | 6.413616e+00 | 8.155377e+00 | 2.116144e+01 | 0.77136 | 0.65311 | 0.45421 |
| S | 6.260184e+00 | 3.565222e+00 | 2.113998e+01 | 0.57693 | 0.28551 | 0.45375 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| H | 7.935501e+00 | 5.997056e+00 | 2.168367e+01 | 0.79049 | 0.48026 | 0.46542 |
| H | 4.790052e+00 | 7.639914e+00 | 2.184305e+01 | 0.63812 | 0.61183 | 0.46884 |
| O | 5.357203e+00 | 8.474370e+00 | 2.192802e+01 | 0.71087 | 0.67865 | 0.47067 |
| C | 3.027834e+00 | 3.954837e+00 | 2.188183e+01 | 0.36835 | 0.31672 | 0.46968 |
| H | 1.007502e+00 | 3.153830e+00 | 2.196542e+01 | 0.19616 | 0.25257 | 0.47147 |
| C | 5.385977e+00 | 4.979092e+00 | 2.196943e+01 | 0.57291 | 0.39874 | 0.47156 |
| C | 1.848827e+00 | 3.531253e+00 | 2.256242e+01 | 0.26962 | 0.28279 | 0.48429 |
| C | 4.137485e+00 | 4.451461e+00 | 2.264201e+01 | 0.46519 | 0.35649 | 0.48599 |
| H | 6.050584e+00 | 5.379284e+00 | 2.276155e+01 | 0.63503 | 0.43079 | 0.48856 |
| C | 1.776835e+00 | 3.553932e+00 | 2.394482e+01 | 0.26554 | 0.28461 | 0.51396 |
| C | 4.048119e+00 | 4.478315e+00 | 2.403119e+01 | 0.46007 | 0.35864 | 0.51581 |
| H | 8.803414e-01 | 3.197274e+00 | 2.447071e+01 | 0.18908 | 0.25605 | 0.52525 |
| H | 4.890375e+00 | 4.857869e+00 | 2.462936e+01 | 0.53368 | 0.38903 | 0.52865 |
| C | 2.885212e+00 | 4.016152e+00 | 2.470833e+01 | 0.36091 | 0.32163 | 0.53035 |
| C | 2.836325e+00 | 3.975778e+00 | 2.611626e+01 | 0.35591 | 0.31839 | 0.56057 |
| C | 2.783851e+00 | 3.875453e+00 | 2.734721e+01 | 0.34825 | 0.31036 | 0.58699 |
| C | 2.786892e+00 | 3.692377e+00 | 2.874166e+01 | 0.34113 | 0.29570 | 0.61692 |
| H | 8.213525e-01 | 2.721426e+00 | 2.885790e+01 | 0.16593 | 0.21794 | 0.61941 |
| H | 4.755786e+00 | 4.598366e+00 | 2.905695e+01 | 0.51396 | 0.36825 | 0.62369 |
| C | 1.706713e+00 | 3.055289e+00 | 2.941639e+01 | 0.24071 | 0.24468 | 0.63140 |
| C | 3.900218e+00 | 4.098765e+00 | 2.953091e+01 | 0.43462 | 0.32824 | 0.63386 |
| C | 1.797402e+00 | 2.840030e+00 | 3.078446e+01 | 0.23838 | 0.22744 | 0.66076 |
| C | 3.898579e+00 | 3.842350e+00 | 3.089421e+01 | 0.42424 | 0.30771 | 0.66312 |
| H | 9.935715e-01 | 2.332980e+00 | 3.133670e+01 | 0.16232 | 0.18683 | 0.67262 |
| H | 4.749540e+00 | 4.128175e+00 | 3.152935e+01 | 0.49470 | 0.33060 | 0.67675 |
| N | 2.872850e+00 | 3.214442e+00 | 3.151887e+01 | 0.32795 | 0.25742 | 0.67653 |
| Au | 2.883758e+00 | 2.913643e+00 | 3.363897e+01 | 0.31667 | 0.23333 | 0.72203 |
| Au | 1.441879e+00 | 2.081173e+00 | 3.599355e+01 | 0.18333 | 0.16667 | 0.77257 |
| Au | 4.325637e+00 | 2.081173e+00 | 3.599355e+01 | 0.38333 | 0.16667 | 0.77257 |
| Au | 2.883758e+00 | 4.578581e+00 | 3.599355e+01 | 0.38333 | 0.36667 | 0.77257 |
| Au | 0.000000e+00 | 1.248704e+00 | 3.834813e+01 | 0.05000 | 0.10000 | 0.82311 |
| Au | 2.883758e+00 | 1.248704e+00 | 3.834813e+01 | 0.25000 | 0.10000 | 0.82311 |
| Au | 5.767516e+00 | 1.248704e+00 | 3.834813e+01 | 0.45000 | 0.10000 | 0.82311 |
| Au | 1.441879e+00 | 3.746112e+00 | 3.834813e+01 | 0.25000 | 0.30000 | 0.82311 |
| Au | 4.325637e+00 | 3.746112e+00 | 3.834813e+01 | 0.45000 | 0.30000 | 0.82311 |
| Au | 2.883758e+00 | 6.243520e+00 | 3.834813e+01 | 0.45000 | 0.50000 | 0.82311 |
| Au | 1.441879e+00 | 4.162346e-01 | 4.070271e+01 | 0.11667 | 0.03333 | 0.87365 |
| Au | 4.325637e+00 | 4.162346e-01 | 4.070271e+01 | 0.31667 | 0.03333 | 0.87365 |
| Au | 7.209396e+00 | 4.162346e-01 | 4.070271e+01 | 0.51667 | 0.03333 | 0.87365 |
| Au | 0.000000e+00 | 2.913643e+00 | 4.070271e+01 | 0.11667 | 0.23333 | 0.87365 |
| Au | 2.883758e+00 | 2.913643e+00 | 4.070271e+01 | 0.31667 | 0.23333 | 0.87365 |
| Au | 5.767516e+00 | 2.913643e+00 | 4.070271e+01 | 0.51667 | 0.23333 | 0.87365 |
| Au | 8.651275e+00 | 2.913643e+00 | 4.070271e+01 | 0.71667 | 0.23333 | 0.87365 |
| Au | -1.441879e+00 | 5.411050e+00 | 4.070271e+01 | 0.11667 | 0.43333 | 0.87365 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 1.441879e+00 | 5.411050e+00 | 4.070271e+01 | 0.31667 | 0.43333 | 0.87365 |
| Au | 4.325637e+00 | 5.411050e+00 | 4.070271e+01 | 0.51667 | 0.43333 | 0.87365 |
| Au | 7.209396e+00 | 5.411050e+00 | 4.070271e+01 | 0.71667 | 0.43333 | 0.87365 |
| Au | 1.009315e+01 | 5.411050e+00 | 4.070271e+01 | 0.91667 | 0.43333 | 0.87365 |
| Au | -0.000000e+00 | 7.908458e+00 | 4.070271e+01 | 0.31667 | 0.63333 | 0.87365 |
| Au | 2.883758e+00 | 7.908458e+00 | 4.070271e+01 | 0.51667 | 0.63333 | 0.87365 |
| Au | 5.767516e+00 | 7.908458e+00 | 4.070271e+01 | 0.71667 | 0.63333 | 0.87365 |
| Au | 8.651275e+00 | 7.908458e+00 | 4.070271e+01 | 0.91667 | 0.63333 | 0.87365 |
| Au | 1.441879e+00 | 1.040587e+01 | 4.070271e+01 | 0.51667 | 0.83333 | 0.87365 |
| Au | 4.325637e+00 | 1.040587e+01 | 4.070271e+01 | 0.71667 | 0.83333 | 0.87365 |
| Au | 7.209396e+00 | 1.040587e+01 | 4.070271e+01 | 0.91667 | 0.83333 | 0.87365 |
| Au | 1.441879e+00 | 2.081173e+00 | 4.305729e+01 | 0.18333 | 0.16667 | 0.92419 |
| Au | 4.325637e+00 | 2.081173e+00 | 4.305729e+01 | 0.38333 | 0.16667 | 0.92419 |
| Au | 7.209396e+00 | 2.081173e+00 | 4.305729e+01 | 0.58333 | 0.16667 | 0.92419 |
| Au | 1.009315e+01 | 2.081173e+00 | 4.305729e+01 | 0.78333 | 0.16667 | 0.92419 |
| Au | 1.297691e+01 | 2.081173e+00 | 4.305729e+01 | 0.98333 | 0.16667 | 0.92419 |
| Au | 0.000000e+00 | 4.578581e+00 | 4.305729e+01 | 0.18333 | 0.36667 | 0.92419 |
| Au | 2.883758e+00 | 4.578581e+00 | 4.305729e+01 | 0.38333 | 0.36667 | 0.92419 |
| Au | 5.767516e+00 | 4.578581e+00 | 4.305729e+01 | 0.58333 | 0.36667 | 0.92419 |
| Au | 8.651275e+00 | 4.578581e+00 | 4.305729e+01 | 0.78333 | 0.36667 | 0.92419 |
| Au | 1.153503e+01 | 4.578581e+00 | 4.305729e+01 | 0.98333 | 0.36667 | 0.92419 |
| Au | -1.441879e+00 | 7.075989e+00 | 4.305729e+01 | 0.18333 | 0.56667 | 0.92419 |
| Au | 1.441879e+00 | 7.075989e+00 | 4.305729e+01 | 0.38333 | 0.56667 | 0.92419 |
| Au | 4.325637e+00 | 7.075989e+00 | 4.305729e+01 | 0.58333 | 0.56667 | 0.92419 |
| Au | 7.209396e+00 | 7.075989e+00 | 4.305729e+01 | 0.78333 | 0.56667 | 0.92419 |
| Au | 1.009315e+01 | 7.075989e+00 | 4.305729e+01 | 0.98333 | 0.56667 | 0.92419 |
| Au | -2.883758e+00 | 9.573397e+00 | 4.305729e+01 | 0.18333 | 0.76667 | 0.92419 |
| Au | 0.000000e+00 | 9.573397e+00 | 4.305729e+01 | 0.38333 | 0.76667 | 0.92419 |
| Au | 2.883758e+00 | 9.573397e+00 | 4.305729e+01 | 0.58333 | 0.76667 | 0.92419 |
| Au | 5.767516e+00 | 9.573397e+00 | 4.305729e+01 | 0.78333 | 0.76667 | 0.92419 |
| Au | 8.651275e+00 | 9.573397e+00 | 4.305729e+01 | 0.98333 | 0.76667 | 0.92419 |
| Au | -4.325637e+00 | 1.207080e+01 | 4.305729e+01 | 0.18333 | 0.96667 | 0.92419 |
| Au | -1.441879e+00 | 1.207080e+01 | 4.305729e+01 | 0.38333 | 0.96667 | 0.92419 |
| Au | 1.441879e+00 | 1.207080e+01 | 4.305729e+01 | 0.58333 | 0.96667 | 0.92419 |
| Au | 4.325637e+00 | 1.207080e+01 | 4.305729e+01 | 0.78333 | 0.96667 | 0.92419 |
| Au | 7.209396e+00 | 1.207080e+01 | 4.305729e+01 | 0.98333 | 0.96667 | 0.92419 |
| Au | 0.000000e+00 | 1.248704e+00 | 4.541187e+01 | 0.05000 | 0.10000 | 0.97473 |
| Au | 2.883758e+00 | 1.248704e+00 | 4.541187e+01 | 0.25000 | 0.10000 | 0.97473 |
| Au | 5.767516e+00 | 1.248704e+00 | 4.541187e+01 | 0.45000 | 0.10000 | 0.97473 |
| Au | 8.651275e+00 | 1.248704e+00 | 4.541187e+01 | 0.65000 | 0.10000 | 0.97473 |
| Au | 1.153503e+01 | 1.248704e+00 | 4.541187e+01 | 0.85000 | 0.10000 | 0.97473 |
| Au | -1.441879e+00 | 3.746112e+00 | 4.541187e+01 | 0.05000 | 0.30000 | 0.97473 |
| Au | 1.441879e+00 | 3.746112e+00 | 4.541187e+01 | 0.25000 | 0.30000 | 0.97473 |
| Au | 4.325637e+00 | 3.746112e+00 | 4.541187e+01 | 0.45000 | 0.30000 | 0.97473 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 7.209396e+00 | 3.746112e+00 | 4.541187e+01 | 0.65000 | 0.30000 | 0.97473 |
| Au | 1.009315e+01 | 3.746112e+00 | 4.541187e+01 | 0.85000 | 0.30000 | 0.97473 |
| Au | -2.883758e+00 | 6.243520e+00 | 4.541187e+01 | 0.05000 | 0.50000 | 0.97473 |
| Au | 0.000000e+00 | 6.243520e+00 | 4.541187e+01 | 0.25000 | 0.50000 | 0.97473 |
| Au | 2.883758e+00 | 6.243520e+00 | 4.541187e+01 | 0.45000 | 0.50000 | 0.97473 |
| Au | 5.767516e+00 | 6.243520e+00 | 4.541187e+01 | 0.65000 | 0.50000 | 0.97473 |
| Au | 8.651275e+00 | 6.243520e+00 | 4.541187e+01 | 0.85000 | 0.50000 | 0.97473 |
| Au | -4.325637e+00 | 8.740928e+00 | 4.541187e+01 | 0.05000 | 0.70000 | 0.97473 |
| Au | -1.441879e+00 | 8.740928e+00 | 4.541187e+01 | 0.25000 | 0.70000 | 0.97473 |
| Au | 1.441879e+00 | 8.740928e+00 | 4.541187e+01 | 0.45000 | 0.70000 | 0.97473 |
| Au | 4.325637e+00 | 8.740928e+00 | 4.541187e+01 | 0.65000 | 0.70000 | 0.97473 |
| Au | 7.209396e+00 | 8.740928e+00 | 4.541187e+01 | 0.85000 | 0.70000 | 0.97473 |
| Au | -5.767516e+00 | 1.123834e+01 | 4.541187e+01 | 0.05000 | 0.90000 | 0.97473 |
| Au | -2.883758e+00 | 1.123834e+01 | 4.541187e+01 | 0.25000 | 0.90000 | 0.97473 |
| Au | 0.000000e+00 | 1.123834e+01 | 4.541187e+01 | 0.45000 | 0.90000 | 0.97473 |
| Au | 2.883758e+00 | 1.123834e+01 | 4.541187e+01 | 0.65000 | 0.90000 | 0.97473 |
| Au | 5.767516e+00 | 1.123834e+01 | 4.541187e+01 | 0.85000 | 0.90000 | 0.97473 |

+-----+

| Left electrode Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

| | | | |
|-------|-----------|-----------|--------------|
| u_1 = | 14.418791 | 0.000000 | 0.000000 Ang |
| u_2 = | -7.209396 | 12.487039 | 0.000000 Ang |
| u_3 = | 0.000000 | 0.000000 | 7.063736 Ang |

+-----+

| Left electrode: Cartesian (Angstrom) / fractional |

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75

Left electrode

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 0.000000e+00 | 1.248704e+00 | 1.177289e+00 | 0.05000 | 0.10000 | 0.16667 |
| Au | 2.883758e+00 | 1.248704e+00 | 1.177289e+00 | 0.25000 | 0.10000 | 0.16667 |
| Au | 5.767516e+00 | 1.248704e+00 | 1.177289e+00 | 0.45000 | 0.10000 | 0.16667 |
| Au | 8.651275e+00 | 1.248704e+00 | 1.177289e+00 | 0.65000 | 0.10000 | 0.16667 |
| Au | 1.153503e+01 | 1.248704e+00 | 1.177289e+00 | 0.85000 | 0.10000 | 0.16667 |
| Au | -1.441879e+00 | 3.746112e+00 | 1.177289e+00 | 0.05000 | 0.30000 | 0.16667 |
| Au | 1.441879e+00 | 3.746112e+00 | 1.177289e+00 | 0.25000 | 0.30000 | 0.16667 |
| Au | 4.325637e+00 | 3.746112e+00 | 1.177289e+00 | 0.45000 | 0.30000 | 0.16667 |
| Au | 7.209396e+00 | 3.746112e+00 | 1.177289e+00 | 0.65000 | 0.30000 | 0.16667 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 1.009315e+01 | 3.746112e+00 | 1.177289e+00 | 0.85000 | 0.30000 | 0.16667 |
| Au | -2.883758e+00 | 6.243520e+00 | 1.177289e+00 | 0.05000 | 0.50000 | 0.16667 |
| Au | -0.000000e+00 | 6.243520e+00 | 1.177289e+00 | 0.25000 | 0.50000 | 0.16667 |
| Au | 2.883758e+00 | 6.243520e+00 | 1.177289e+00 | 0.45000 | 0.50000 | 0.16667 |
| Au | 5.767516e+00 | 6.243520e+00 | 1.177289e+00 | 0.65000 | 0.50000 | 0.16667 |
| Au | 8.651275e+00 | 6.243520e+00 | 1.177289e+00 | 0.85000 | 0.50000 | 0.16667 |
| Au | -4.325637e+00 | 8.740928e+00 | 1.177289e+00 | 0.05000 | 0.70000 | 0.16667 |
| Au | -1.441879e+00 | 8.740928e+00 | 1.177289e+00 | 0.25000 | 0.70000 | 0.16667 |
| Au | 1.441879e+00 | 8.740928e+00 | 1.177289e+00 | 0.45000 | 0.70000 | 0.16667 |
| Au | 4.325637e+00 | 8.740928e+00 | 1.177289e+00 | 0.65000 | 0.70000 | 0.16667 |
| Au | 7.209396e+00 | 8.740928e+00 | 1.177289e+00 | 0.85000 | 0.70000 | 0.16667 |
| Au | -5.767516e+00 | 1.123834e+01 | 1.177289e+00 | 0.05000 | 0.90000 | 0.16667 |
| Au | -2.883758e+00 | 1.123834e+01 | 1.177289e+00 | 0.25000 | 0.90000 | 0.16667 |
| Au | -0.000000e+00 | 1.123834e+01 | 1.177289e+00 | 0.45000 | 0.90000 | 0.16667 |
| Au | 2.883758e+00 | 1.123834e+01 | 1.177289e+00 | 0.65000 | 0.90000 | 0.16667 |
| Au | 5.767516e+00 | 1.123834e+01 | 1.177289e+00 | 0.85000 | 0.90000 | 0.16667 |
| Au | 1.441879e+00 | 2.081173e+00 | 3.531868e+00 | 0.18333 | 0.16667 | 0.50000 |
| Au | 4.325637e+00 | 2.081173e+00 | 3.531868e+00 | 0.38333 | 0.16667 | 0.50000 |
| Au | 7.209396e+00 | 2.081173e+00 | 3.531868e+00 | 0.58333 | 0.16667 | 0.50000 |
| Au | 1.009315e+01 | 2.081173e+00 | 3.531868e+00 | 0.78333 | 0.16667 | 0.50000 |
| Au | 1.297691e+01 | 2.081173e+00 | 3.531868e+00 | 0.98333 | 0.16667 | 0.50000 |
| Au | -0.000000e+00 | 4.578581e+00 | 3.531868e+00 | 0.18333 | 0.36667 | 0.50000 |
| Au | 2.883758e+00 | 4.578581e+00 | 3.531868e+00 | 0.38333 | 0.36667 | 0.50000 |
| Au | 5.767516e+00 | 4.578581e+00 | 3.531868e+00 | 0.58333 | 0.36667 | 0.50000 |
| Au | 8.651275e+00 | 4.578581e+00 | 3.531868e+00 | 0.78333 | 0.36667 | 0.50000 |
| Au | 1.153503e+01 | 4.578581e+00 | 3.531868e+00 | 0.98333 | 0.36667 | 0.50000 |
| Au | -1.441879e+00 | 7.075989e+00 | 3.531868e+00 | 0.18333 | 0.56667 | 0.50000 |
| Au | 1.441879e+00 | 7.075989e+00 | 3.531868e+00 | 0.38333 | 0.56667 | 0.50000 |
| Au | 4.325637e+00 | 7.075989e+00 | 3.531868e+00 | 0.58333 | 0.56667 | 0.50000 |
| Au | 7.209396e+00 | 7.075989e+00 | 3.531868e+00 | 0.78333 | 0.56667 | 0.50000 |
| Au | 1.009315e+01 | 7.075989e+00 | 3.531868e+00 | 0.98333 | 0.56667 | 0.50000 |
| Au | -2.883758e+00 | 9.573397e+00 | 3.531868e+00 | 0.18333 | 0.76667 | 0.50000 |
| Au | -0.000000e+00 | 9.573397e+00 | 3.531868e+00 | 0.38333 | 0.76667 | 0.50000 |
| Au | 2.883758e+00 | 9.573397e+00 | 3.531868e+00 | 0.58333 | 0.76667 | 0.50000 |
| Au | 5.767516e+00 | 9.573397e+00 | 3.531868e+00 | 0.78333 | 0.76667 | 0.50000 |
| Au | 8.651275e+00 | 9.573397e+00 | 3.531868e+00 | 0.98333 | 0.76667 | 0.50000 |
| Au | -4.325637e+00 | 1.207080e+01 | 3.531868e+00 | 0.18333 | 0.96667 | 0.50000 |
| Au | -1.441879e+00 | 1.207080e+01 | 3.531868e+00 | 0.38333 | 0.96667 | 0.50000 |
| Au | 1.441879e+00 | 1.207080e+01 | 3.531868e+00 | 0.58333 | 0.96667 | 0.50000 |
| Au | 4.325637e+00 | 1.207080e+01 | 3.531868e+00 | 0.78333 | 0.96667 | 0.50000 |
| Au | 7.209396e+00 | 1.207080e+01 | 3.531868e+00 | 0.98333 | 0.96667 | 0.50000 |
| Au | 1.441879e+00 | 4.162346e-01 | 5.886447e+00 | 0.11667 | 0.03333 | 0.83333 |
| Au | 4.325637e+00 | 4.162346e-01 | 5.886447e+00 | 0.31667 | 0.03333 | 0.83333 |
| Au | 7.209396e+00 | 4.162346e-01 | 5.886447e+00 | 0.51667 | 0.03333 | 0.83333 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 1.009315e+01 | 4.162346e-01 | 5.886447e+00 | 0.71667 | 0.03333 | 0.83333 |
| Au | 1.297691e+01 | 4.162346e-01 | 5.886447e+00 | 0.91667 | 0.03333 | 0.83333 |
| Au | -0.000000e+00 | 2.913643e+00 | 5.886447e+00 | 0.11667 | 0.23333 | 0.83333 |
| Au | 2.883758e+00 | 2.913643e+00 | 5.886447e+00 | 0.31667 | 0.23333 | 0.83333 |
| Au | 5.767516e+00 | 2.913643e+00 | 5.886447e+00 | 0.51667 | 0.23333 | 0.83333 |
| Au | 8.651275e+00 | 2.913643e+00 | 5.886447e+00 | 0.71667 | 0.23333 | 0.83333 |
| Au | 1.153503e+01 | 2.913643e+00 | 5.886447e+00 | 0.91667 | 0.23333 | 0.83333 |
| Au | -1.441879e+00 | 5.411050e+00 | 5.886447e+00 | 0.11667 | 0.43333 | 0.83333 |
| Au | 1.441879e+00 | 5.411050e+00 | 5.886447e+00 | 0.31667 | 0.43333 | 0.83333 |
| Au | 4.325637e+00 | 5.411050e+00 | 5.886447e+00 | 0.51667 | 0.43333 | 0.83333 |
| Au | 7.209396e+00 | 5.411050e+00 | 5.886447e+00 | 0.71667 | 0.43333 | 0.83333 |
| Au | 1.009315e+01 | 5.411050e+00 | 5.886447e+00 | 0.91667 | 0.43333 | 0.83333 |
| Au | -2.883758e+00 | 7.908458e+00 | 5.886447e+00 | 0.11667 | 0.63333 | 0.83333 |
| Au | -0.000000e+00 | 7.908458e+00 | 5.886447e+00 | 0.31667 | 0.63333 | 0.83333 |
| Au | 2.883758e+00 | 7.908458e+00 | 5.886447e+00 | 0.51667 | 0.63333 | 0.83333 |
| Au | 5.767516e+00 | 7.908458e+00 | 5.886447e+00 | 0.71667 | 0.63333 | 0.83333 |
| Au | 8.651275e+00 | 7.908458e+00 | 5.886447e+00 | 0.91667 | 0.63333 | 0.83333 |
| Au | -4.325637e+00 | 1.040587e+01 | 5.886447e+00 | 0.11667 | 0.83333 | 0.83333 |
| Au | -1.441879e+00 | 1.040587e+01 | 5.886447e+00 | 0.31667 | 0.83333 | 0.83333 |
| Au | 1.441879e+00 | 1.040587e+01 | 5.886447e+00 | 0.51667 | 0.83333 | 0.83333 |
| Au | 4.325637e+00 | 1.040587e+01 | 5.886447e+00 | 0.71667 | 0.83333 | 0.83333 |
| Au | 7.209396e+00 | 1.040587e+01 | 5.886447e+00 | 0.91667 | 0.83333 | 0.83333 |

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| Right electrode Bravais lattice |

+-----+

Type:

UnitCell

Lattice constants:

Primitive vectors:

u_1 = 14.418791 0.000000 0.000000 Ang

u_2 = -7.209396 12.487039 0.000000 Ang

u_3 = 0.000000 0.000000 7.063736 Ang

+-----+

| Right electrode: Cartesian (Angstrom) / fractional |

+-----+

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Right electrode

| | | | | | | |
|----|--------------|--------------|--------------|---------|---------|---------|
| Au | 1.441879e+00 | 4.162346e-01 | 1.177311e+00 | 0.11667 | 0.03333 | 0.16667 |
| Au | 4.325637e+00 | 4.162346e-01 | 1.177311e+00 | 0.31667 | 0.03333 | 0.16667 |
| Au | 7.209396e+00 | 4.162346e-01 | 1.177311e+00 | 0.51667 | 0.03333 | 0.16667 |
| Au | 0.000000e+00 | 2.913643e+00 | 1.177311e+00 | 0.11667 | 0.23333 | 0.16667 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 2.883758e+00 | 2.913643e+00 | 1.177311e+00 | 0.31667 | 0.23333 | 0.16667 |
| Au | 5.767516e+00 | 2.913643e+00 | 1.177311e+00 | 0.51667 | 0.23333 | 0.16667 |
| Au | 8.651275e+00 | 2.913643e+00 | 1.177311e+00 | 0.71667 | 0.23333 | 0.16667 |
| Au | -1.441879e+00 | 5.411050e+00 | 1.177311e+00 | 0.11667 | 0.43333 | 0.16667 |
| Au | 1.441879e+00 | 5.411050e+00 | 1.177311e+00 | 0.31667 | 0.43333 | 0.16667 |
| Au | 4.325637e+00 | 5.411050e+00 | 1.177311e+00 | 0.51667 | 0.43333 | 0.16667 |
| Au | 7.209396e+00 | 5.411050e+00 | 1.177311e+00 | 0.71667 | 0.43333 | 0.16667 |
| Au | 1.009315e+01 | 5.411050e+00 | 1.177311e+00 | 0.91667 | 0.43333 | 0.16667 |
| Au | -0.000000e+00 | 7.908458e+00 | 1.177311e+00 | 0.31667 | 0.63333 | 0.16667 |
| Au | 2.883758e+00 | 7.908458e+00 | 1.177311e+00 | 0.51667 | 0.63333 | 0.16667 |
| Au | 5.767516e+00 | 7.908458e+00 | 1.177311e+00 | 0.71667 | 0.63333 | 0.16667 |
| Au | 8.651275e+00 | 7.908458e+00 | 1.177311e+00 | 0.91667 | 0.63333 | 0.16667 |
| Au | 1.441879e+00 | 1.040587e+01 | 1.177311e+00 | 0.51667 | 0.83333 | 0.16667 |
| Au | 4.325637e+00 | 1.040587e+01 | 1.177311e+00 | 0.71667 | 0.83333 | 0.16667 |
| Au | 7.209396e+00 | 1.040587e+01 | 1.177311e+00 | 0.91667 | 0.83333 | 0.16667 |
| Au | 1.441879e+00 | 2.081173e+00 | 3.531889e+00 | 0.18333 | 0.16667 | 0.50000 |
| Au | 4.325637e+00 | 2.081173e+00 | 3.531889e+00 | 0.38333 | 0.16667 | 0.50000 |
| Au | 7.209396e+00 | 2.081173e+00 | 3.531889e+00 | 0.58333 | 0.16667 | 0.50000 |
| Au | 1.009315e+01 | 2.081173e+00 | 3.531889e+00 | 0.78333 | 0.16667 | 0.50000 |
| Au | 1.297691e+01 | 2.081173e+00 | 3.531889e+00 | 0.98333 | 0.16667 | 0.50000 |
| Au | 0.000000e+00 | 4.578581e+00 | 3.531889e+00 | 0.18333 | 0.36667 | 0.50000 |
| Au | 2.883758e+00 | 4.578581e+00 | 3.531889e+00 | 0.38333 | 0.36667 | 0.50000 |
| Au | 5.767516e+00 | 4.578581e+00 | 3.531889e+00 | 0.58333 | 0.36667 | 0.50000 |
| Au | 8.651275e+00 | 4.578581e+00 | 3.531889e+00 | 0.78333 | 0.36667 | 0.50000 |
| Au | 1.153503e+01 | 4.578581e+00 | 3.531889e+00 | 0.98333 | 0.36667 | 0.50000 |
| Au | -1.441879e+00 | 7.075989e+00 | 3.531889e+00 | 0.18333 | 0.56667 | 0.50000 |
| Au | 1.441879e+00 | 7.075989e+00 | 3.531889e+00 | 0.38333 | 0.56667 | 0.50000 |
| Au | 4.325637e+00 | 7.075989e+00 | 3.531889e+00 | 0.58333 | 0.56667 | 0.50000 |
| Au | 7.209396e+00 | 7.075989e+00 | 3.531889e+00 | 0.78333 | 0.56667 | 0.50000 |
| Au | 1.009315e+01 | 7.075989e+00 | 3.531889e+00 | 0.98333 | 0.56667 | 0.50000 |
| Au | -2.883758e+00 | 9.573397e+00 | 3.531889e+00 | 0.18333 | 0.76667 | 0.50000 |
| Au | 0.000000e+00 | 9.573397e+00 | 3.531889e+00 | 0.38333 | 0.76667 | 0.50000 |
| Au | 2.883758e+00 | 9.573397e+00 | 3.531889e+00 | 0.58333 | 0.76667 | 0.50000 |
| Au | 5.767516e+00 | 9.573397e+00 | 3.531889e+00 | 0.78333 | 0.76667 | 0.50000 |
| Au | 8.651275e+00 | 9.573397e+00 | 3.531889e+00 | 0.98333 | 0.76667 | 0.50000 |
| Au | -4.325637e+00 | 1.207080e+01 | 3.531889e+00 | 0.18333 | 0.96667 | 0.50000 |
| Au | -1.441879e+00 | 1.207080e+01 | 3.531889e+00 | 0.38333 | 0.96667 | 0.50000 |
| Au | 1.441879e+00 | 1.207080e+01 | 3.531889e+00 | 0.58333 | 0.96667 | 0.50000 |
| Au | 4.325637e+00 | 1.207080e+01 | 3.531889e+00 | 0.78333 | 0.96667 | 0.50000 |
| Au | 7.209396e+00 | 1.207080e+01 | 3.531889e+00 | 0.98333 | 0.96667 | 0.50000 |
| Au | 0.000000e+00 | 1.248704e+00 | 5.886468e+00 | 0.05000 | 0.10000 | 0.83334 |
| Au | 2.883758e+00 | 1.248704e+00 | 5.886468e+00 | 0.25000 | 0.10000 | 0.83334 |
| Au | 5.767516e+00 | 1.248704e+00 | 5.886468e+00 | 0.45000 | 0.10000 | 0.83334 |
| Au | 8.651275e+00 | 1.248704e+00 | 5.886468e+00 | 0.65000 | 0.10000 | 0.83334 |

| | | | | | | |
|----|---------------|--------------|--------------|---------|---------|---------|
| Au | 1.153503e+01 | 1.248704e+00 | 5.886468e+00 | 0.85000 | 0.10000 | 0.83334 |
| Au | -1.441879e+00 | 3.746112e+00 | 5.886468e+00 | 0.05000 | 0.30000 | 0.83334 |
| Au | 1.441879e+00 | 3.746112e+00 | 5.886468e+00 | 0.25000 | 0.30000 | 0.83334 |
| Au | 4.325637e+00 | 3.746112e+00 | 5.886468e+00 | 0.45000 | 0.30000 | 0.83334 |
| Au | 7.209396e+00 | 3.746112e+00 | 5.886468e+00 | 0.65000 | 0.30000 | 0.83334 |
| Au | 1.009315e+01 | 3.746112e+00 | 5.886468e+00 | 0.85000 | 0.30000 | 0.83334 |
| Au | -2.883758e+00 | 6.243520e+00 | 5.886468e+00 | 0.05000 | 0.50000 | 0.83334 |
| Au | 0.000000e+00 | 6.243520e+00 | 5.886468e+00 | 0.25000 | 0.50000 | 0.83334 |
| Au | 2.883758e+00 | 6.243520e+00 | 5.886468e+00 | 0.45000 | 0.50000 | 0.83334 |
| Au | 5.767516e+00 | 6.243520e+00 | 5.886468e+00 | 0.65000 | 0.50000 | 0.83334 |
| Au | 8.651275e+00 | 6.243520e+00 | 5.886468e+00 | 0.85000 | 0.50000 | 0.83334 |
| Au | -4.325637e+00 | 8.740928e+00 | 5.886468e+00 | 0.05000 | 0.70000 | 0.83334 |
| Au | -1.441879e+00 | 8.740928e+00 | 5.886468e+00 | 0.25000 | 0.70000 | 0.83334 |
| Au | 1.441879e+00 | 8.740928e+00 | 5.886468e+00 | 0.45000 | 0.70000 | 0.83334 |
| Au | 4.325637e+00 | 8.740928e+00 | 5.886468e+00 | 0.65000 | 0.70000 | 0.83334 |
| Au | 7.209396e+00 | 8.740928e+00 | 5.886468e+00 | 0.85000 | 0.70000 | 0.83334 |
| Au | -5.767516e+00 | 1.123834e+01 | 5.886468e+00 | 0.05000 | 0.90000 | 0.83334 |
| Au | -2.883758e+00 | 1.123834e+01 | 5.886468e+00 | 0.25000 | 0.90000 | 0.83334 |
| Au | 0.000000e+00 | 1.123834e+01 | 5.886468e+00 | 0.45000 | 0.90000 | 0.83334 |
| Au | 2.883758e+00 | 1.123834e+01 | 5.886468e+00 | 0.65000 | 0.90000 | 0.83334 |
| Au | 5.767516e+00 | 1.123834e+01 | 5.886468e+00 | 0.85000 | 0.90000 | 0.83334 |

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