

Electron transport through molecular wires based on a face-shared bioctahedral motif.

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Supporting information

- 1) Optimized Cartesian coordinates and total energies of the gas-phase species $[\text{Rh}_2\text{Cl}_9]^{3-}$, $[\text{Ru}_2\text{Cl}_9]^{3-}$ and $[\text{Mo}_2\text{Cl}_9]^{3-}$
- 2) Cartesian coordinates of the scattering regions used in the two-probe calculations.

Structures and energies of the optimized complexes

$[\text{Mo}_2\text{Cl}_9]^{3-}$ Energy = -51.52367518 eV

Cl	-2.021172	0.000000	2.555442
Cl	1.010586	1.750386	2.555442
Cl	1.010586	-1.750386	2.555442
Mo	0.000000	0.000000	1.192181
Cl	-1.097133	1.900290	-0.000279
Cl	-1.097133	-1.900290	-0.000279
Cl	2.194266	0.000000	-0.000279
Mo	0.000000	0.000000	-1.190164
Cl	-2.020067	0.000000	-2.555836
Cl	1.010034	1.749429	-2.555836
Cl	1.010034	-1.749429	-2.555836

$[\text{Ru}_2\text{Cl}_9]^{3-}$ Energy = -45.40247651 eV

Cl	-1.950056	0.000000	-2.722447
Cl	0.975028	-1.688798	-2.722447
Cl	0.975028	1.688798	-2.722447
Ru	0.000000	0.000000	-1.362434
Cl	-0.970874	-1.681603	0.000148
Cl	-0.970874	1.681603	0.000148
Cl	1.941748	0.000000	0.000148
Ru	0.000000	0.000000	1.362540
Cl	-1.950228	0.000000	2.722265
Cl	0.975114	-1.688947	2.722265
Cl	0.975114	1.688947	2.722265

$[\text{Rh}_2\text{Cl}_9]^{3-}$ Energy = -42.29992309 eV

Cl	-1.932148	0.000000	-2.919055
Cl	0.966074	-1.673289	-2.919055
Cl	0.966074	1.673289	-2.919055
Rh	0.000000	0.000000	-1.584081
Cl	-0.893213	-1.547090	0.000032
Cl	-0.893213	1.547090	0.000032
Cl	1.786426	0.000000	0.000032
Rh	0.000000	0.000000	1.584068
Cl	-1.932166	0.000000	2.919029
Cl	0.966083	-1.673305	2.919029
Cl	0.966083	1.673305	2.919029

Coordinates of central regions used in ATK 2010 calculations:

[Mo₂Cl₉]³⁻ M-M = 2.38 Angstrom

Au 2.58499996e-08, 4.16234647e-01, 1.17731000e+00
Au 5.76751649e+00, 4.16234647e-01, 1.17731000e+00
Au 8.65127472e+00, 4.16234647e-01, 1.17731000e+00
Au 1.15350329e+01, 4.16234647e-01, 1.17731000e+00
Au 2.88375826e+00, 4.16234647e-01, 1.17731000e+00
Au 4.32563738e+00, 2.91364253e+00, 1.17731000e+00
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Cl 6.07537514e+00, 5.23328986e+00, 1.29502100e+01
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Cl 4.32563453e+00, 4.04936349e+00, 1.55058430e+01
Cl 2.42545453e+00, 7.34057180e+00, 1.55058430e+01
Mo 4.32563502e+00, 6.24350265e+00, 1.66970040e+01
Cl 6.07537514e+00, 5.23328986e+00, 1.80614760e+01
Cl 4.32563514e+00, 8.26392844e+00, 1.80614760e+01
Cl 2.57589564e+00, 5.23329015e+00, 1.80614760e+01
Au -2.88375820e+00, 8.74092759e+00, 2.04160751e+01
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Au 1.44187915e+00, 1.12383355e+01, 2.74798113e+01
Au 1.15350329e+01, 3.74611182e+00, 2.74798113e+01
Au 5.76751650e+00, 3.74611182e+00, 2.74798113e+01
Au 7.20939561e+00, 7.90845830e+00, 2.98343900e+01
Au -1.44187909e+00, 2.91364253e+00, 2.98343900e+01
Au -2.88375820e+00, 1.04058662e+01, 2.98343900e+01
Au 2.88375826e+00, 5.41105041e+00, 2.98343900e+01
Au 5.76751649e+00, 1.04058662e+01, 2.98343900e+01
Au 2.58500000e-08, 4.16234647e-01, 2.98343900e+01
Au -2.88375820e+00, 5.41105041e+00, 2.98343900e+01
Au 1.44187915e+00, 2.91364253e+00, 2.98343900e+01
Au -4.32563732e+00, 7.90845830e+00, 2.98343900e+01
Au 4.32563738e+00, 2.91364253e+00, 2.98343900e+01
Au 2.58299950e-08, 1.04058662e+01, 2.98343900e+01
Au 8.65127472e+00, 4.16234647e-01, 2.98343900e+01
Au 1.15350329e+01, 4.16234647e-01, 2.98343900e+01
Au 5.76751649e+00, 5.41105041e+00, 2.98343900e+01
Au 4.32563738e+00, 7.90845830e+00, 2.98343900e+01
Au 1.00931538e+01, 2.91364253e+00, 2.98343900e+01
Au 2.88375826e+00, 1.04058662e+01, 2.98343900e+01
Au 7.20939561e+00, 2.91364253e+00, 2.98343900e+01
Au 5.76751649e+00, 4.16234647e-01, 2.98343900e+01
Au -5.76751643e+00, 1.04058662e+01, 2.98343900e+01
Au -1.44187909e+00, 7.90845830e+00, 2.98343900e+01
Au 2.58399995e-08, 5.41105041e+00, 2.98343900e+01
Au 2.88375826e+00, 4.16234647e-01, 2.98343900e+01
Au 8.65127472e+00, 5.41105041e+00, 2.98343900e+01
Au 1.44187915e+00, 7.90845830e+00, 2.98343900e+01

[Mo₂Cl₉]³⁻ M-M = 2.83 Angstrom

Au 2.58499996e-08, 4.16234647e-01, 1.17731000e+00

Au 5.76751649e+00, 4.16234647e-01, 1.17731000e+00
Au 8.65127472e+00, 4.16234647e-01, 1.17731000e+00
Au 2.88375826e+00, 4.16234647e-01, 1.17731000e+00
Au 1.15350329e+01, 4.16234647e-01, 1.17731000e+00
Au 2.58399999e-08, 5.41105041e+00, 1.17731000e+00
Au 7.20939561e+00, 2.91364253e+00, 1.17731000e+00
Au -2.88375820e+00, 5.41105041e+00, 1.17731000e+00
Au 5.76751649e+00, 5.41105041e+00, 1.17731000e+00
Au 1.00931538e+01, 2.91364253e+00, 1.17731000e+00
Au 4.32563738e+00, 2.91364253e+00, 1.17731000e+00
Au 8.65127472e+00, 5.41105041e+00, 1.17731000e+00
Au 1.44187915e+00, 2.91364253e+00, 1.17731000e+00
Au -1.44187909e+00, 2.91364253e+00, 1.17731000e+00
Au 2.88375826e+00, 5.41105041e+00, 1.17731000e+00
Au 7.20939561e+00, 7.90845830e+00, 1.17731000e+00
Au -1.44187909e+00, 7.90845830e+00, 1.17731000e+00
Au 4.32563738e+00, 7.90845830e+00, 1.17731000e+00
Au 1.44187915e+00, 7.90845830e+00, 1.17731000e+00
Au -4.32563732e+00, 7.90845830e+00, 1.17731000e+00
Au -5.76751643e+00, 1.04058662e+01, 1.17731000e+00
Au -2.88375820e+00, 1.04058662e+01, 1.17731000e+00
Au 5.76751649e+00, 1.04058662e+01, 1.17731000e+00
Au 2.88375826e+00, 1.04058662e+01, 1.17731000e+00
Au 2.58299968e-08, 1.04058662e+01, 1.17731000e+00
Au 3.06599968e-08, 3.74611182e+00, 3.53188874e+00
Au 1.29769120e+01, 1.24870394e+00, 3.53188874e+00
Au 1.15350329e+01, 3.74611182e+00, 3.53188874e+00
Au 5.76751650e+00, 3.74611182e+00, 3.53188874e+00
Au 7.20939561e+00, 1.24870394e+00, 3.53188874e+00
Au 8.65127473e+00, 3.74611182e+00, 3.53188874e+00
Au 1.00931538e+01, 1.24870394e+00, 3.53188874e+00
Au 4.32563738e+00, 1.24870394e+00, 3.53188874e+00
Au 1.44187915e+00, 1.24870394e+00, 3.53188874e+00
Au 2.88375827e+00, 3.74611182e+00, 3.53188874e+00
Au -2.88375820e+00, 8.74092759e+00, 3.53188874e+00
Au 4.32563738e+00, 1.12383355e+01, 3.53188874e+00
Au 1.00931538e+01, 6.24351971e+00, 3.53188874e+00
Au 1.44187915e+00, 1.12383355e+01, 3.53188874e+00
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Au 5.76751650e+00, 8.74092759e+00, 3.53188874e+00
Au 7.20939561e+00, 1.12383355e+01, 3.53188874e+00
Au -4.32563731e+00, 1.12383355e+01, 3.53188874e+00
Au 1.44187915e+00, 6.24351971e+00, 3.53188874e+00
Au 7.20939561e+00, 6.24351971e+00, 3.53188874e+00
Au 3.06499963e-08, 8.74092759e+00, 3.53188874e+00
Au 8.65127473e+00, 8.74092759e+00, 3.53188874e+00
Au 1.44187915e+00, 4.57858112e+00, 5.88646747e+00
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Au 1.15350329e+01, 2.08117323e+00, 5.88646747e+00
Au -2.88375820e+00, 7.07598900e+00, 5.88646747e+00
Au 7.20939561e+00, 4.57858112e+00, 5.88646747e+00

Au 8.65127472e+00, 2.08117323e+00, 5.88646747e+00
Au 8.65127472e+00, 7.07598900e+00, 5.88646747e+00
Au 2.88375826e+00, 7.07598900e+00, 5.88646747e+00
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Au -4.32563732e+00, 9.57339689e+00, 5.88646747e+00
Au 2.88375826e+00, 1.20708048e+01, 5.88646747e+00
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Au 2.58299986e-08, 1.20708048e+01, 5.88646747e+00
Au 5.76751649e+00, 1.20708048e+01, 5.88646747e+00
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Au 7.20939561e+00, 9.57339689e+00, 5.88646747e+00
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Au 2.88375826e+00, 1.04058662e+01, 8.24104621e+00
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Au 4.32563738e+00, 2.91364253e+00, 8.24104621e+00
Au 8.65127472e+00, 5.41105041e+00, 8.24104621e+00
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Au 1.15350329e+01, 4.16234647e-01, 8.24104621e+00
Au 1.00931538e+01, 2.91364253e+00, 8.24104621e+00
Au 5.76751649e+00, 4.16234647e-01, 8.24104621e+00
Au 4.32563738e+00, 7.90845830e+00, 8.24104621e+00
Au 1.44187915e+00, 7.90845830e+00, 8.24104621e+00
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Au 1.15350329e+01, 3.74611182e+00, 1.05956250e+01
Au 2.88375827e+00, 3.74611182e+00, 1.05956250e+01
Au 3.06499963e-08, 8.74092759e+00, 1.05956250e+01
Au 8.65127473e+00, 8.74092759e+00, 1.05956250e+01
Au 4.32563738e+00, 6.24351971e+00, 1.05956250e+01
Au 1.00931538e+01, 6.24351971e+00, 1.05956250e+01
Au 7.20939561e+00, 1.24870394e+00, 1.05956250e+01
Au 2.88375827e+00, 8.74092759e+00, 1.05956250e+01
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Au 7.20939561e+00, 6.24351971e+00, 1.05956250e+01
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Au -4.32563731e+00, 1.12383355e+01, 1.05956250e+01
Au 5.76751650e+00, 3.74611182e+00, 1.05956250e+01
Au 3.06599972e-08, 3.74611182e+00, 1.05956250e+01
Cl 2.59556707e+00, 5.24465821e+00, 1.29502400e+01
Cl 4.32563818e+00, 8.24122915e+00, 1.29502400e+01
Cl 6.05570918e+00, 5.24465827e+00, 1.29502400e+01
Mo 4.32563815e+00, 6.24351521e+00, 1.43505110e+01
Cl 6.06616041e+00, 7.24840621e+00, 1.57651660e+01
Cl 4.32563801e+00, 4.23373344e+00, 1.57651660e+01
Cl 2.58511601e+00, 7.24840598e+00, 1.57651660e+01
Mo 4.32563815e+00, 6.24351521e+00, 1.71798210e+01
Cl 6.05570918e+00, 5.24465827e+00, 1.85800920e+01
Cl 4.32563818e+00, 8.24122915e+00, 1.85800920e+01
Cl 2.59556707e+00, 5.24465821e+00, 1.85800920e+01
Au -2.88375820e+00, 8.74092759e+00, 2.09346751e+01
Au 3.06599968e-08, 3.74611182e+00, 2.09346751e+01
Au 2.88375827e+00, 8.74092759e+00, 2.09346751e+01
Au 8.65127473e+00, 8.74092759e+00, 2.09346751e+01
Au 7.20939561e+00, 1.24870394e+00, 2.09346751e+01
Au 1.00931538e+01, 1.24870394e+00, 2.09346751e+01
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Au 7.20939561e+00, 2.91364253e+00, 2.32892538e+01
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Au 2.58299968e-08, 1.04058662e+01, 2.32892538e+01
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Au 2.58499993e-08, 4.16234647e-01, 2.32892538e+01
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Au 4.32563738e+00, 9.57339689e+00, 2.56438325e+01
Au -1.44187909e+00, 9.57339689e+00, 2.56438325e+01
Au 1.29769120e+01, 1.24870394e+00, 2.79984113e+01
Au 2.88375827e+00, 3.74611182e+00, 2.79984113e+01
Au 1.44187915e+00, 1.24870394e+00, 2.79984113e+01
Au 4.32563738e+00, 1.24870394e+00, 2.79984113e+01
Au -2.88375820e+00, 8.74092759e+00, 2.79984113e+01
Au -4.32563731e+00, 1.12383355e+01, 2.79984113e+01

Au 8.65127473e+00, 8.74092759e+00, 2.79984113e+01
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Au -1.44187908e+00, 1.12383355e+01, 2.79984113e+01
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Au 1.15350329e+01, 3.74611182e+00, 2.79984113e+01
Au 5.76751650e+00, 3.74611182e+00, 2.79984113e+01
Au 7.20939561e+00, 7.90845830e+00, 3.03529900e+01
Au -1.44187909e+00, 2.91364253e+00, 3.03529900e+01
Au -2.88375820e+00, 1.04058662e+01, 3.03529900e+01
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Au 5.76751649e+00, 1.04058662e+01, 3.03529900e+01
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Au -2.88375820e+00, 5.41105041e+00, 3.03529900e+01
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Au 4.32563738e+00, 7.90845830e+00, 3.03529900e+01
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Au 8.65127472e+00, 5.41105041e+00, 3.03529900e+01
Au 1.44187915e+00, 7.90845830e+00, 3.03529900e+01

[Ru₂Cl₉]³⁻

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Au 4.32563738e+00, 1.24870394e+00, 2.07515751e+01
Au 2.88375827e+00, 8.74092759e+00, 2.07515751e+01
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Au 5.76751650e+00, 3.74611182e+00, 2.78153113e+01
Au 7.20939561e+00, 7.90845830e+00, 3.01698900e+01
Au -1.44187909e+00, 2.91364253e+00, 3.01698900e+01
Au -2.88375820e+00, 1.04058662e+01, 3.01698900e+01
Au 2.88375826e+00, 5.41105041e+00, 3.01698900e+01
Au 5.76751649e+00, 1.04058662e+01, 3.01698900e+01
Au 2.58500000e-08, 4.16234647e-01, 3.01698900e+01
Au -2.88375820e+00, 5.41105041e+00, 3.01698900e+01
Au 1.44187915e+00, 2.91364253e+00, 3.01698900e+01
Au -4.32563732e+00, 7.90845830e+00, 3.01698900e+01
Au 4.32563738e+00, 2.91364253e+00, 3.01698900e+01
Au 2.58299950e-08, 1.04058662e+01, 3.01698900e+01
Au 8.65127472e+00, 4.16234647e-01, 3.01698900e+01
Au 1.15350329e+01, 4.16234647e-01, 3.01698900e+01
Au 5.76751649e+00, 5.41105041e+00, 3.01698900e+01
Au 4.32563738e+00, 7.90845830e+00, 3.01698900e+01
Au 1.00931538e+01, 2.91364253e+00, 3.01698900e+01
Au 2.88375826e+00, 1.04058662e+01, 3.01698900e+01
Au 7.20939561e+00, 2.91364253e+00, 3.01698900e+01
Au 5.76751649e+00, 4.16234647e-01, 3.01698900e+01
Au -5.76751643e+00, 1.04058662e+01, 3.01698900e+01
Au -1.44187909e+00, 7.90845830e+00, 3.01698900e+01
Au 2.58399995e-08, 5.41105041e+00, 3.01698900e+01
Au 2.88375826e+00, 4.16234647e-01, 3.01698900e+01
Au 8.65127472e+00, 5.41105041e+00, 3.01698900e+01
Au 1.44187915e+00, 7.90845830e+00, 3.01698900e+01

[Rh₂Cl₉]³⁻

Au 2.58499996e-08, 4.16234647e-01, 1.17731000e+00
Au 5.76751649e+00, 4.16234647e-01, 1.17731000e+00
Au 8.65127472e+00, 4.16234647e-01, 1.17731000e+00
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Au 2.88375826e+00, 4.16234647e-01, 1.17731000e+00
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Au 8.65127472e+00, 5.41105041e+00, 1.17731000e+00
Au 1.44187915e+00, 2.91364253e+00, 1.17731000e+00
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Au 1.00931538e+01, 2.91364253e+00, 1.17731000e+00
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Au 2.58399999e-08, 5.41105041e+00, 1.17731000e+00

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Au 7.20939561e+00, 2.91364253e+00, 1.17731000e+00
Au 1.44187915e+00, 7.90845830e+00, 1.17731000e+00
Au 4.32563738e+00, 7.90845830e+00, 1.17731000e+00
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Au 2.58299968e-08, 1.04058662e+01, 1.17731000e+00
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Au 1.29769120e+01, 1.24870394e+00, 3.53188874e+00
Au 1.44187915e+00, 1.12383355e+01, 3.53188874e+00
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Au 8.65127473e+00, 8.74092759e+00, 1.05956250e+01
Au 1.00931538e+01, 6.24351971e+00, 1.05956250e+01
Au 7.20939561e+00, 1.24870394e+00, 1.05956250e+01
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Au 4.32563738e+00, 1.24870394e+00, 1.05956250e+01
Au 5.76751650e+00, 8.74092759e+00, 1.05956250e+01
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Cl 4.32559134e+00, 8.17555968e+00, 1.29502000e+01
Cl 2.65239612e+00, 5.27750081e+00, 1.29502000e+01
Rh 4.32559098e+00, 6.24352031e+00, 1.42852620e+01
Cl 5.87287526e+00, 7.13684531e+00, 1.58692450e+01
Cl 2.77830633e+00, 7.13684592e+00, 1.58692450e+01
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Rh 4.32559098e+00, 6.24352031e+00, 1.74532280e+01
Cl 2.65239612e+00, 5.27750081e+00, 1.87882900e+01
Cl 4.32559134e+00, 8.17555968e+00, 1.87882900e+01
Cl 5.99878634e+00, 5.27750093e+00, 1.87882900e+01
Au 1.15350329e+01, 3.74611182e+00, 2.11428751e+01
Au 3.06599968e-08, 3.74611182e+00, 2.11428751e+01
Au 4.32563738e+00, 1.24870394e+00, 2.11428751e+01
Au 2.88375827e+00, 8.74092759e+00, 2.11428751e+01
Au -2.88375820e+00, 8.74092759e+00, 2.11428751e+01
Au 1.00931538e+01, 6.24351971e+00, 2.11428751e+01
Au 4.32563738e+00, 6.24351971e+00, 2.11428751e+01
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Au -1.44187908e+00, 6.24351971e+00, 2.11428751e+01
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Au 8.65127473e+00, 8.74092759e+00, 2.82066113e+01
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Au 7.20939561e+00, 1.12383355e+01, 2.82066113e+01
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Au -1.44187908e+00, 1.12383355e+01, 2.82066113e+01

Au 1.00931538e+01, 1.24870394e+00, 2.82066113e+01
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Au 5.76751650e+00, 3.74611182e+00, 2.82066113e+01
Au 7.20939561e+00, 7.90845830e+00, 3.05611900e+01
Au -1.44187909e+00, 2.91364253e+00, 3.05611900e+01
Au -2.88375820e+00, 1.04058662e+01, 3.05611900e+01
Au 2.88375826e+00, 5.41105041e+00, 3.05611900e+01
Au 5.76751649e+00, 1.04058662e+01, 3.05611900e+01
Au 2.58500000e-08, 4.16234647e-01, 3.05611900e+01
Au -2.88375820e+00, 5.41105041e+00, 3.05611900e+01
Au 1.44187915e+00, 2.91364253e+00, 3.05611900e+01
Au -4.32563732e+00, 7.90845830e+00, 3.05611900e+01
Au 4.32563738e+00, 2.91364253e+00, 3.05611900e+01
Au 2.58299950e-08, 1.04058662e+01, 3.05611900e+01
Au 8.65127472e+00, 4.16234647e-01, 3.05611900e+01
Au 1.15350329e+01, 4.16234647e-01, 3.05611900e+01
Au 5.76751649e+00, 5.41105041e+00, 3.05611900e+01
Au 4.32563738e+00, 7.90845830e+00, 3.05611900e+01
Au 1.00931538e+01, 2.91364253e+00, 3.05611900e+01
Au 2.88375826e+00, 1.04058662e+01, 3.05611900e+01
Au 7.20939561e+00, 2.91364253e+00, 3.05611900e+01
Au 5.76751649e+00, 4.16234647e-01, 3.05611900e+01
Au -5.76751643e+00, 1.04058662e+01, 3.05611900e+01
Au -1.44187909e+00, 7.90845830e+00, 3.05611900e+01
Au 2.58399995e-08, 5.41105041e+00, 3.05611900e+01
Au 2.88375826e+00, 4.16234647e-01, 3.05611900e+01
Au 8.65127472e+00, 5.41105041e+00, 3.05611900e+01
Au 1.44187915e+00, 7.90845830e+00, 3.05611900e+01