SUPPORTING INFORMATION

Three Sites Molecular Orbital Controlled Single-Molecule Rectifier based on Perpendicularly Linked Porphyrin-Imide Dyads

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Method

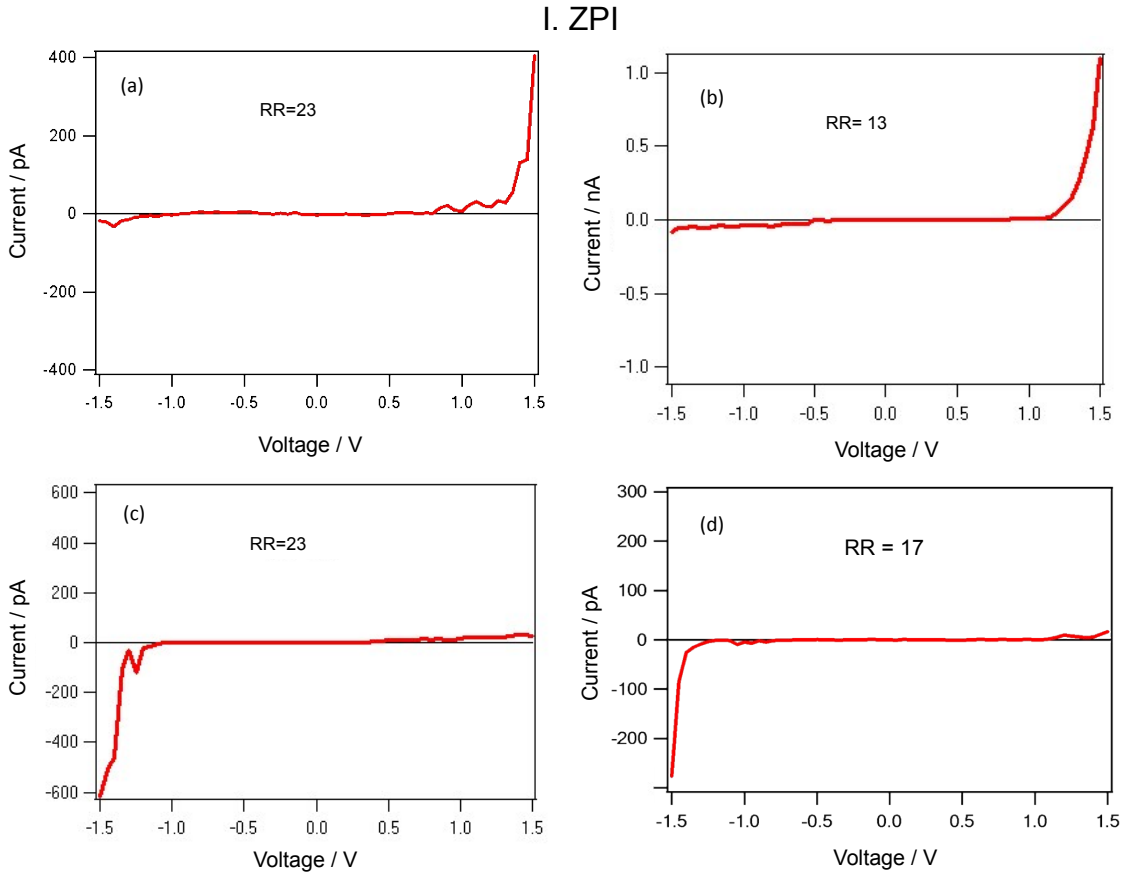
The single-molecule conductance of ZPI and RPI was obtained using an STM break junction (BJ) with Molecular Imaging Picoscan, Picoscan 5.3.3 software. A single-crystalline gold surface Au(111) on mica substrate was prepared by flame annealing. After that, the dilute solution of the sample with a concentration of about 1 mM in acetone solvent was immersed for one night. The gold STM tip from Au wire (99.99% and diameter of 0.25 nm) was cut and placed at the tip holder of STM-BJ. During the STM-BJ measurements, the Au tip was repeatedly brought into and out of contact with the substrate at room temperature. The conductance of the molecule was determined from the conductance histogram, which was built from thousands of conductance traces measured during the breaking process with an applied bias of 500 mV between the tip and substrate.

I-V curve measurements were conducted using mechanically controllable break junctions (MCBJ). The measurements were carried out using Au (50 nm)/Cr (5 nm) electrodes with a spacing of ~1 μm; the electrodes were prepared by conventional photolithography combined with the lift-off technique on a thin phosphor bronze substrate (thickness: 100 μm) covered by an insulated layer of polyimide. The spacing between the electrodes was reduced to establish contact by the electrodeposition of gold using a commercial solution (TEMPEREX 8400, Electroplating Engineers of Japan Ltd.). More details are provided in Supporting Information (Fig. S3). The diode molecules (ZPI or RPI) and the symmetric molecule were dissolved in acetone (~1 mM) and deposited on the electrodes. Measurements were carried out in vacuum at 300 K using an Agilent B1500A semiconductor device analyzer with high-resolution source measurement units. For each molecule, 6 electrodes were used and ca. 30 molecule junctions were successfully made to measure total ca. 500 *I-V* scans.

Because the molecule diodes in the experiments had the same linker groups (–OH groups) for both ends, the orientation of molecules in the junction during MCBJ measurements could not be controlled, and two different orientations of ZPI and RPI should have been present between the two electrodes. Figure S1 displays typical individual *I–V* curves of ZPI (Fig. S1a and b) and RPI (Fig. S1c and d), which are reasonably assigned to the molecules with different orientations. Here, we refer to the results, which show a higher conductance at positive bias as the forward orientation. Although from a statistical perspective, both directions should be observed equally, the probability

of achieving a forward orientation was higher, simply because we set the instrumentations at +1.5 V (positive bias) to observe the expected conductance from the histogram. Ideally, the histograms shown in Fig. 1 should have two peaks corresponding to the forward and backward orientations. However, because of the very low conductance for the reversed bias, the smaller peaks could not be observed with the present instrumental setup.

I-V curves measurement and Individual I–V curves of metal porphyrin–imide single-molecule diodes



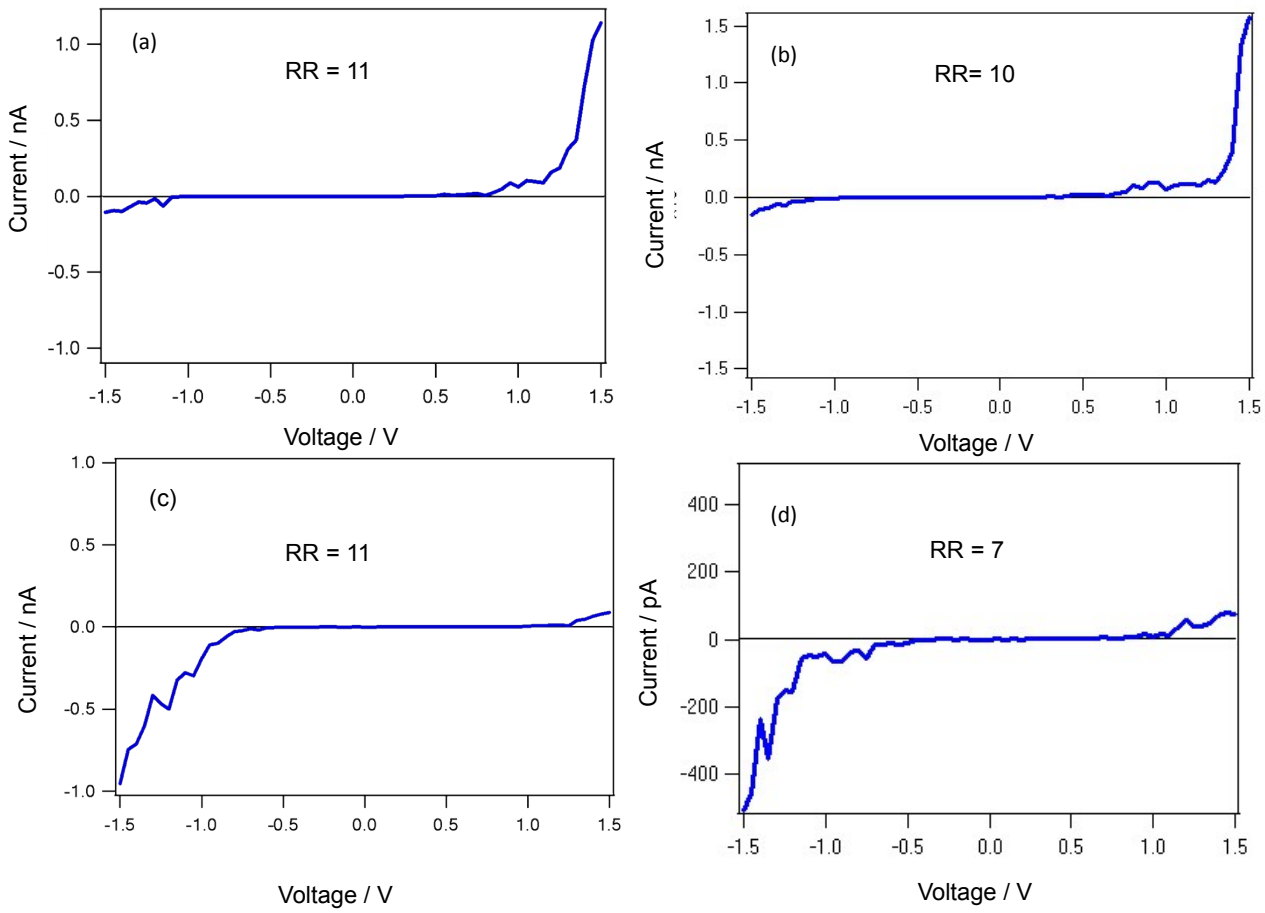


Figure S1. Typical individual *I–V* curves of ZPI (I) and RPI (II).

Forward orientation and backward orientation of ZPI (red lines) and RPI (blue lines) are shown. The RR values corresponding to the selected individual *I–V* curve of ZPI for the forward orientations are 23 and 13, and those for the backward orientations are 23 and 17. The RR values of forward orientations for RPI are 11 and 10, and those for the backward orientations are 11 and 7.

2D conductance histogram of ZPI and RPI and the selected individual traces

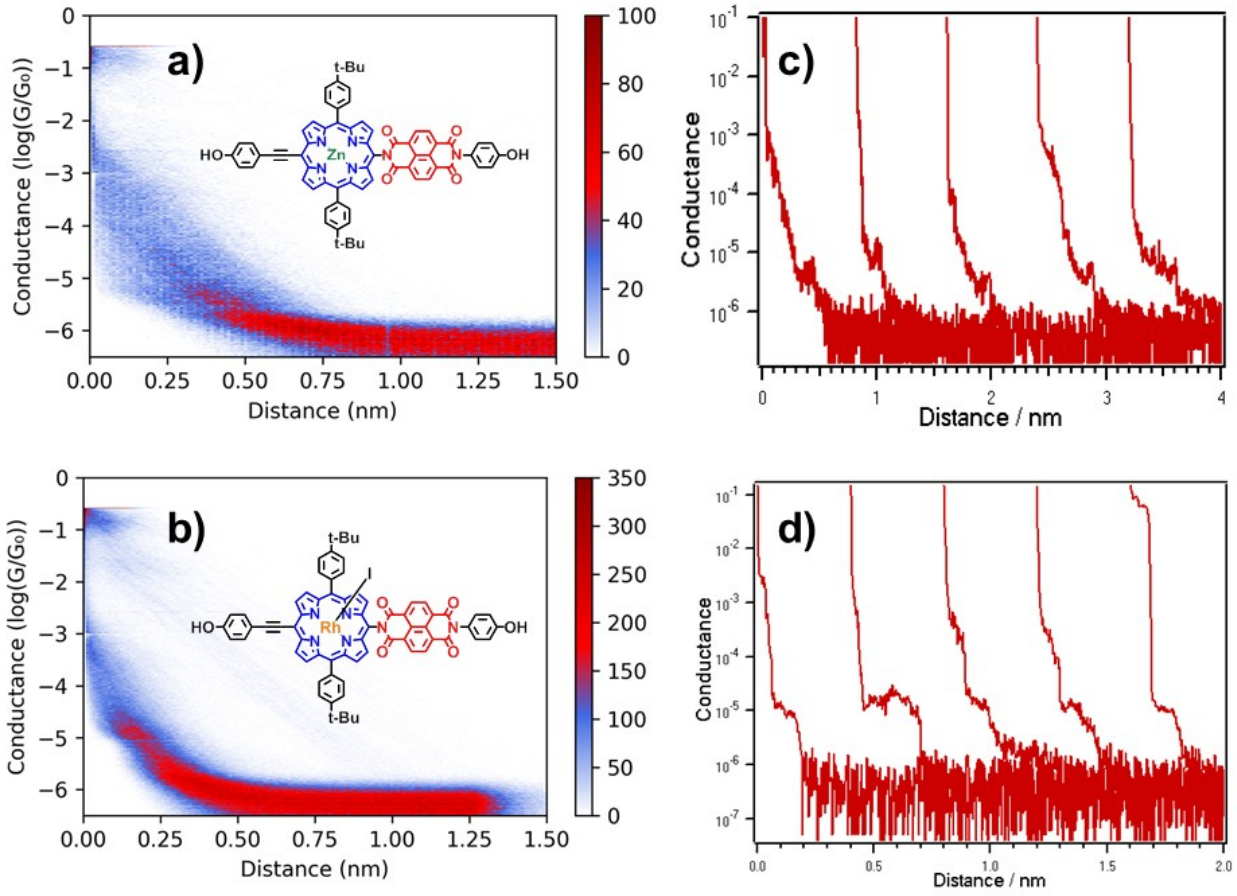


Figure S2. (a) 2D Conductance histograms for ZPI constructed obtained from 1767 measurements of individual traces. (b) 2D Conductance histograms for RPI constructed from 4070 measurements of individual traces. Insets: structure of ZPI and RPI. (c-d) Selected individual traces of ZPI and RPI respectively

Conductance histogram of Acetone

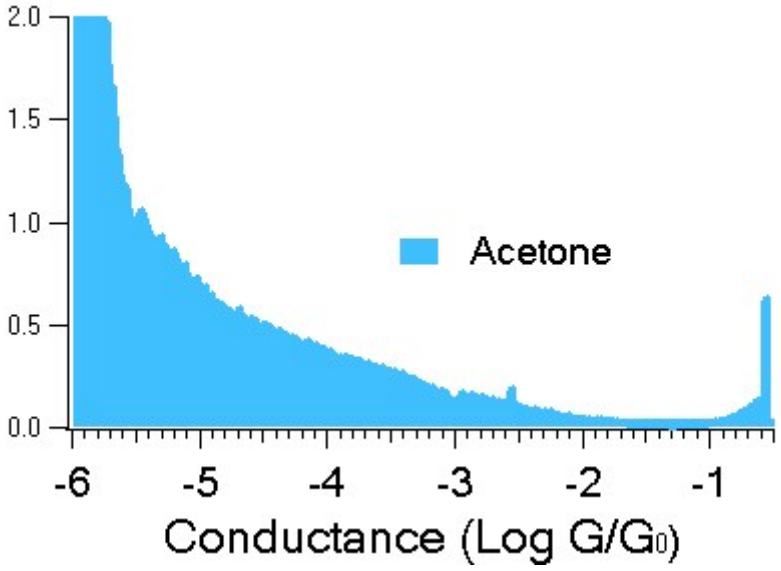


Figure S3. Conductance histogram of acetone solvent. It is seen that there is no peak observed in the conductance histogram

Conductance histogram of symmetric ZnII-5,15-di(4-hydorxyphenyl)porphyrin

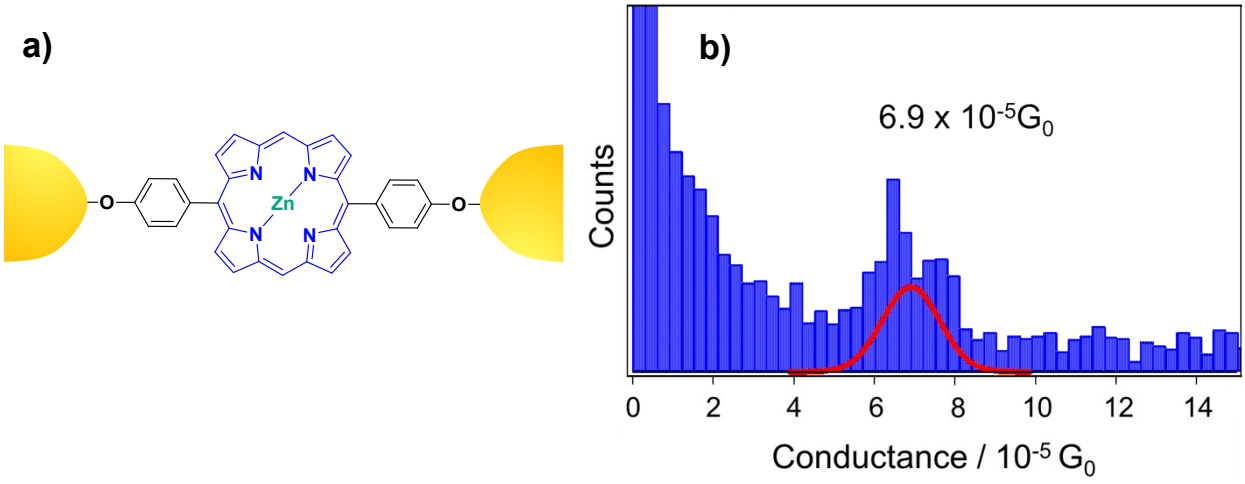


Figure S4. Molecular structure and conductance histogram of the symmetric porphyrin molecule Zn^{II}-5,15-bis(4-hydorxyphenyl)porphyrin (ZHPP).

a) Single-molecule junction of Au–symmetric-molecule–Au. b) Conductance histogram of the symmetric molecule ZHPP ; the maximum conductance was 6.9 × 10-5 G_0.

Electrode Fabrication

The electrodes used for MCBJ measurements were patterned by photolithography on a substrate made of phosphor bronze covered with an insulating polyimide film. The photolithographic processes were performed at room temperature. A Cr/Au (5nm/50nm) layer was first formed on the substrate using electron-beam vapor deposition followed by treatment with lift-off solvents (60% dimethyl sulfoxide, 40% *N*-methyl-2-pyrrolidone). The size of the electrode gaps, measuring ~1 μm, were reduced by electroplating using a gold solution until gap contacts were established. Scanning electron microscope (SEM) images of the gaps are displayed at Fig. S5.

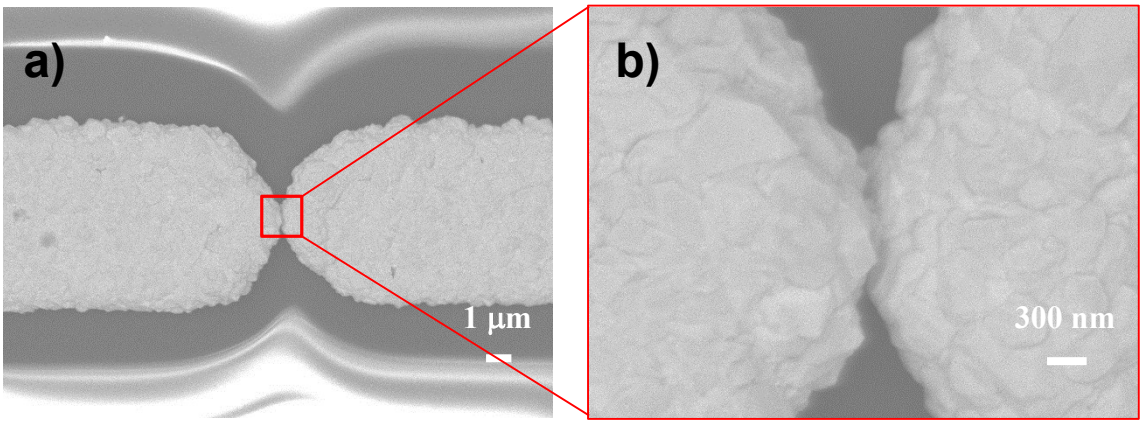


Figure S5. SEM images of the electrodes after electroplating. a) Gold electrodes after electroplating. b) Enlarged view of the area framed by the red rectangle in a).

Gas phase DFT calculation

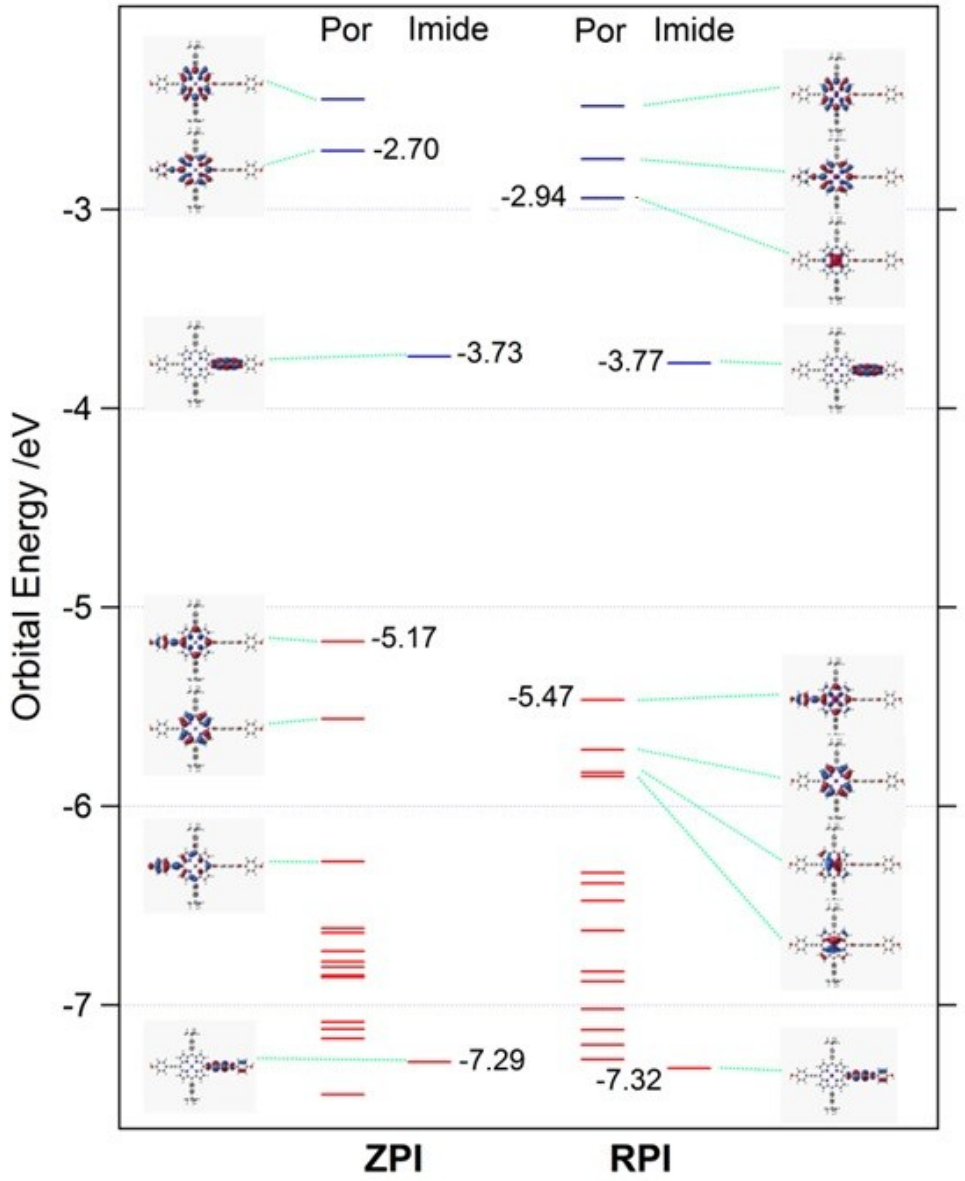


Figure S6. Molecular orbital energy alignment of ZPI and RPI. The molecular orbitals were calculated using the functional / basis set B3LYP/6-311G of the program Gaussian 09.

NEGF-DFT calculation

The transport properties of the molecules were calculated by using the SMEAGOL code[1-3] based on the SIESTA package.[4] SMEAGOL employs the nonequilibrium Green's function method combined with density functional theory (NEGF-DFT). Double and single zeta plus polarization basis set was used for the molecule and Au atoms, respectively. Core electrons were described by the Troullier-Martins norm-conserving pseudopotential[5] with the Kleinman-Bylander nonlocal projector.[6] We used the Perdew-Burke-Ernzerhof (PBE)[7] exchange-correlation functional. The electrode was modeled as au Au(111) slab having $p(6\times6)$ periodicity with the tip-like electrode surfaces as shown in Fig. S5. The oxygen atom is placed at the hollow site of the Au(111) surface. After the structures of the molecule and topmost two layers are optimized, we added the electrode layers and performed transport calculations.[9] The k-points were sampled by a 2×2×1 grid for the structural optimization and electronic structures and by an 8×8×1 grid for the transmission function and molecular projected self-consistent Hamiltonian (MPSH)[9] analysis. The positions of molecular orbitals in Figure 3 are extracted from the MPSH analysis under the finite bias.

Figure S8 shows the transmission functions of ZPI and RPI. Two curves are very similar but the small difference in the energy level alignment can be seen. The calculated zero-bias conductance is 1.2×10^{-5} G_0 and 7.0×10^{-6} G_0, respectively. The slightly large conductance of ZPI is consistent with the higher HOMO level of ZPI shown in Fig. S6. The difference in the magnitude relation of the conductance values still remains to be resolved in future work. It is also known that the PBE functional predicts the porphyrin HOMO that is very close to the Fermi level of the Au electrode.[8] The higher threshold bias voltages predicted by the present NEGF-DFT calculations would be attributed to this error.

Figure S9 shows the bias dependent transmission functions for ZPI and RPI. The peak heights are very small at 0 V because the all MOs are localized, while sharp peaks due to resonance can be observed at high bias. The properties of peaks are summarized in Table S1.

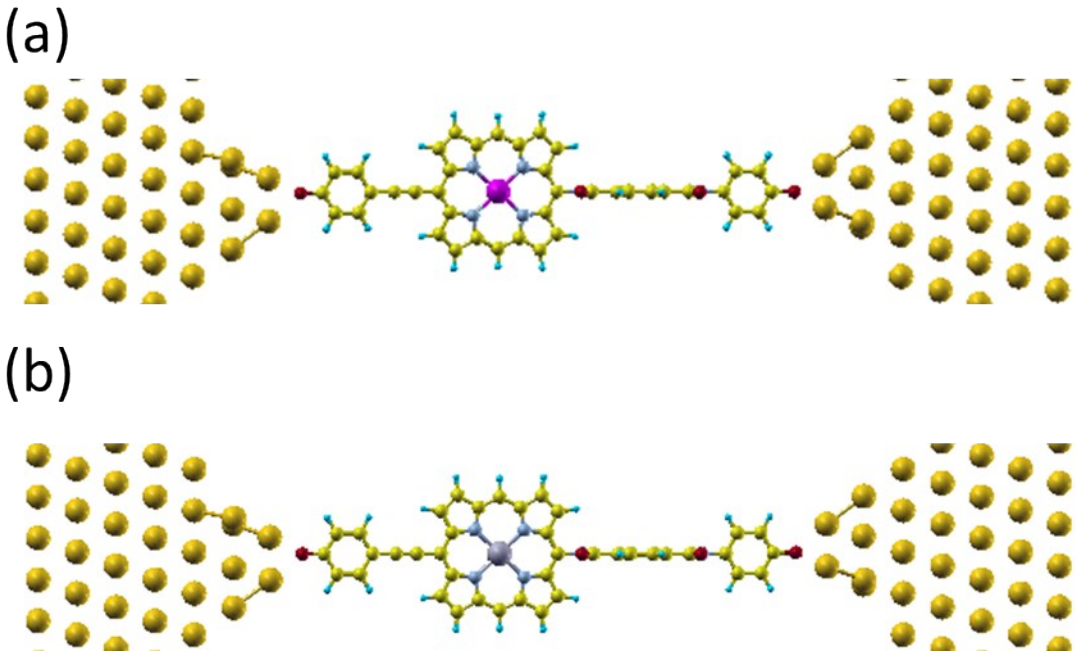


Figure S7. Molecular junction structures of (a)Au-ZPI-Au and (b)Au-RPI-Au.

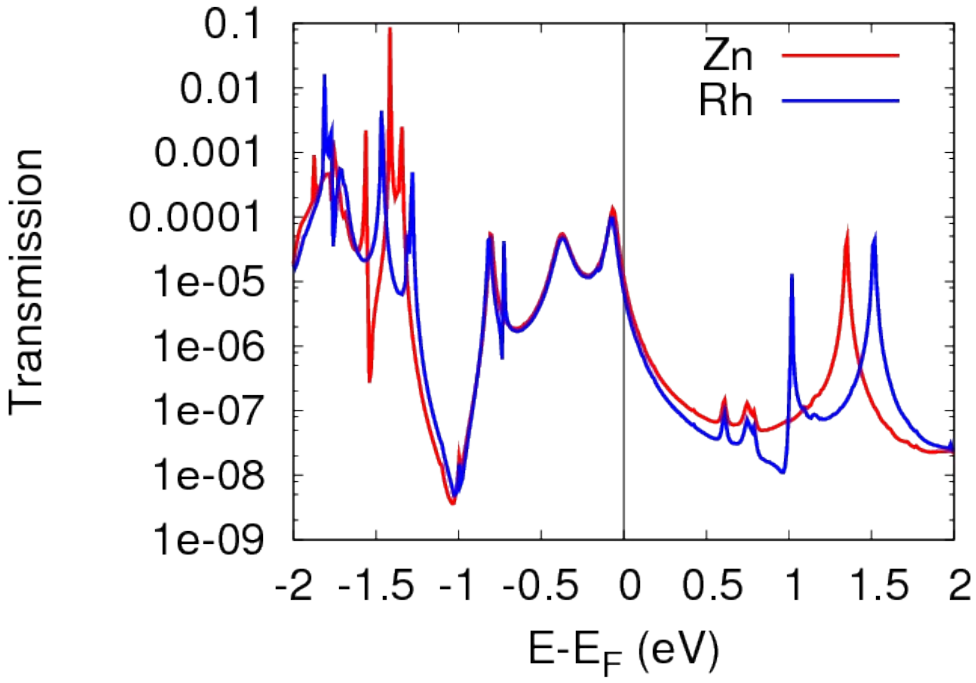


Figure S8. Transmission functions.

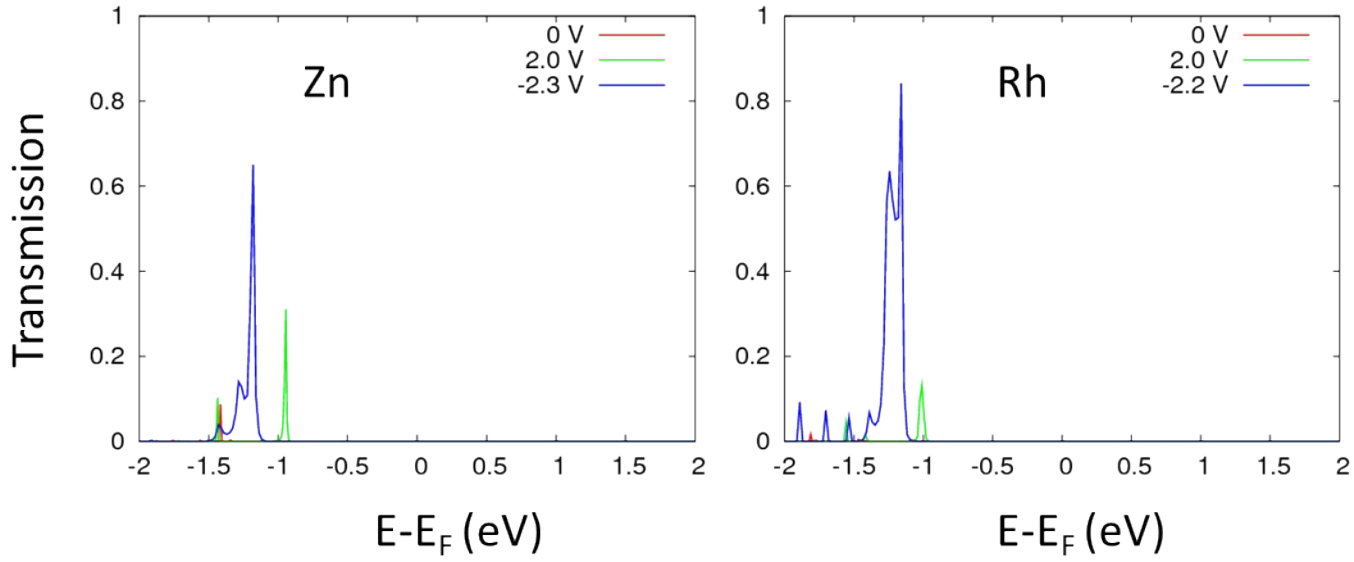


Figure S9. Bias dependent transmission functions.

Table S1. Properties of the resonance molecular orbitals. The position of the MO with respect to the Fermi level (E_{MO}), the transmission value at E_{MO} ($T(E_{MO})$), and the coupling product, where $\gamma_{L/R}$ is the coupling between the MO and the left/right electrode.

	Zn			Rh		
Bias (V)	E_{MO} (eV)	$T(E_{MO})$ (G_0)	$\sqrt{\gamma_L\gamma_R}$ (meV)	E_{MO} (eV)	$T(E_{MO})$ (G_0)	$\sqrt{\gamma_L\gamma_R}$ (meV)
-2.3	-1.18	0.65	10.7	-1.16	0.84	14.7
2.0	-0.95	0.31	5.3	-1.01	0.13	3.6
2.4				-1.13	0.19	4.1

Three-site model analysis

To investigate the possibility to improve the rectification ratio (RR) of our molecules, we constructed a three-site model. The voltage-dependent Hamiltonian of this model is given as

$$H(V) = \begin{pmatrix} \varepsilon_1 + z + \alpha_1 eV & -t_{12} & 0 \\ -t_{12} & \varepsilon_2 + z + \alpha_2 e|V| & -t_{23} \\ 0 & -t_{23} & \varepsilon_3 + \alpha_3 eV \end{pmatrix}, \quad \text{(S1)}$$

where V is the applied voltage, e the electron charge, ε the molecular orbital energy with respect to the Fermi energy, and t the coupling between orbitals. z is a variable to shift molecular orbitals of porphyrin and imide parts (we assume that those two parts are easier to be chemically modified). The retarted Green's function is given as

$$G^r(\varepsilon,V) = \left(\varepsilon I - H(V) - \Sigma_L - \Sigma_R\right)^{-1}, \quad \text{(S2)}$$

where $\Sigma_{L,R}$ are the self-energy matrices representing the left and right electrodes. By ignoring the real part of the self-energy (energy shift due to the coupling to the electrodes) and energy dependence of the coupling (wide-band limit), $\Sigma_{L,R}$ can be simplified to

$$\Sigma_L = \begin{pmatrix} -i\Gamma/2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Sigma_R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -i\Gamma/2 \end{pmatrix}. \quad \text{(S3)}$$

Within the NEGF formalism, the transmission function $T(\varepsilon,V)$ is given as

$$T(\varepsilon,V) = Tr[\Gamma_L G^r(\varepsilon,V)\Gamma_R G^a(\varepsilon,V)], \quad \text{(S4)}$$

Where $G^r = G^{a\,\dagger}$ and $\Gamma_{L/R} = i(\Sigma_{L/R} - \Sigma_{L/R}^{\dagger})$. We calculated the current as

$$I(V) = \frac{2e}{h}\int_{-eV/2}^{+eV/2} T(\varepsilon,V)d\varepsilon. \quad \text{(S5)}$$

Based on the NEGF-DFT results for ZPI, we set the parameters as follows: ε_1= −0.6 eV, ε_2= −1.35 eV, ε_3= −0.41 eV, α_1= −0.45, α_2= 0.2, α_3= 0.15, t_{12}=t_{23}= 0.03 eV, and Γ= 0.1 eV. The calculated current-voltage (*IV*) characteristic is shown in Figure S10 well reproduced the *IV* curve calculated from NEGF-DFT: (i) the sharp rise of the current at around +2 V, (ii) very small but non-negligible peak at around +0.5 V, and (iii) the rise of the current at large negative bias due to the non-linear voltage dependence of ε_2.

It has been indicated that the RR decreases rapidly for increasing the misalignment between the resonant orbital and the Fermi level.[10] As shown in Figure 3(c) in the main text, the energy of the resonance (ε_{res}) is −0.9 eV for ZPI, which is away from the Fermi level. We calculated $RR = I(V_{max})/I(-V_{max})$, where V_{max} is the voltage where the current becomes the maximum, by changing the *z* value from 0 eV to 0.9 eV, which corresponds to changing ε_{res} from −0.9 eV to 0 eV. Figure S11 shows that, based on the three-site model, the RR of the *IV* curve shown in Figure S10 is ~5 and the maximum RR of ~420 can be achieved by shifting the energy levels of molecular orbitals. This maximum RR is smaller than that (~10^6) predicted from a multi-site model,[10] because the current at the negative voltage due to the $|V|$ dependence of ε_2, which was not considered in the previous model, reduces the RR.

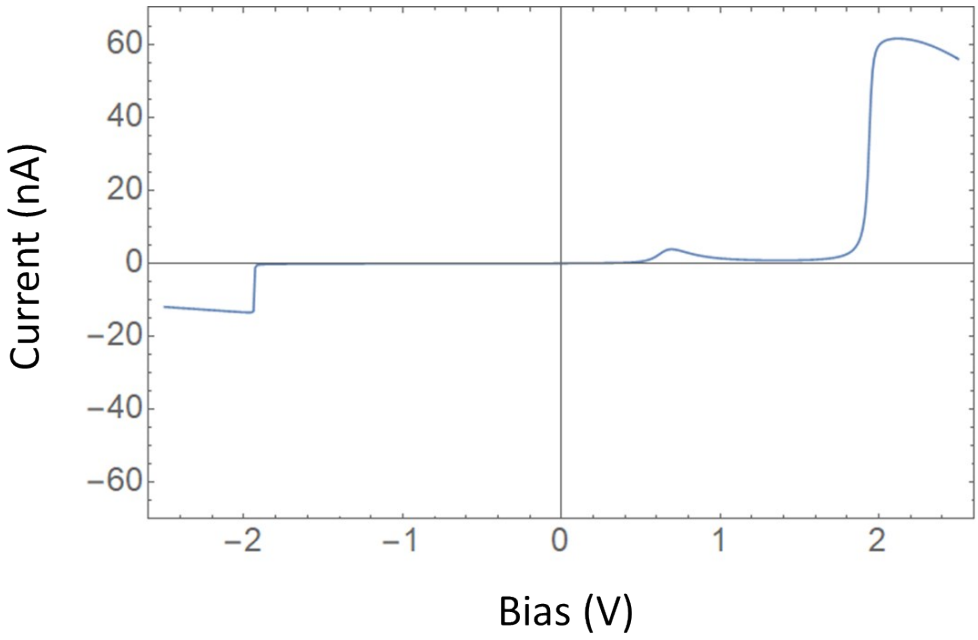


Figure S10. Current-voltage (*IV*) characteristic using the three-site model (z=0).

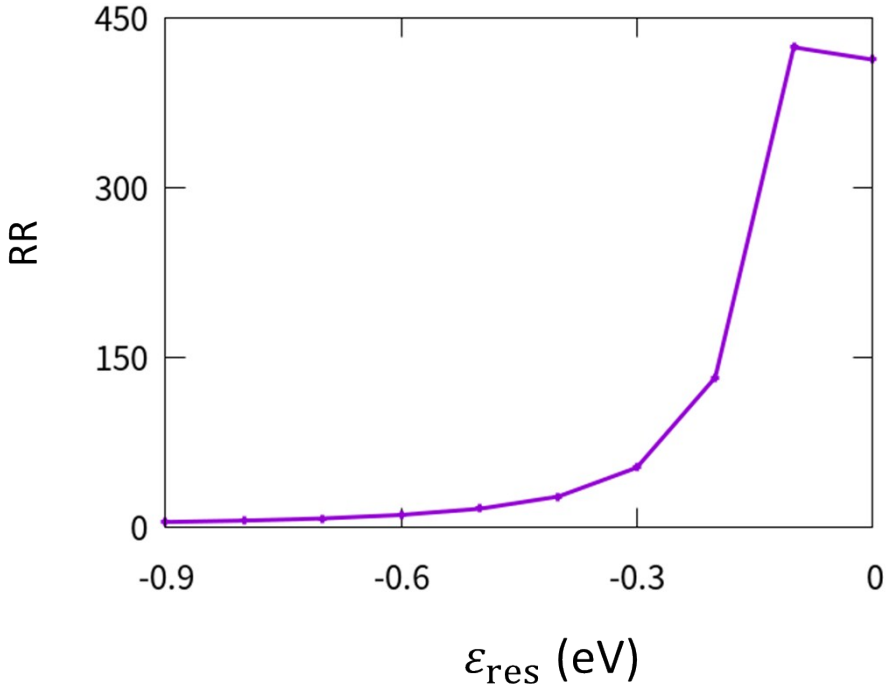
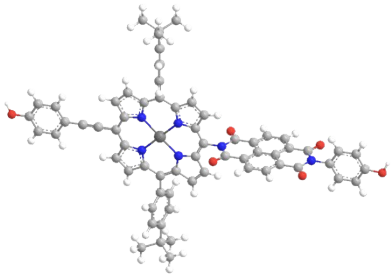


Figure S11. RR calculated by changing ε_{res} from −0.9 eV (z = 0 eV) to 0 eV (z = 0.9 eV).

Dihedral Angle Dependence of Energy Porphyrin-imide Molecule



Gaussian 09, DFT, B3LYP, 6-311G.

Boltzmann distribution:

$$P_A \propto e^{-\frac{E_{rel}}{RT}}$$

Where P_A is the probability of conformation with dihedral A, E_{rel} is the relative energy in J/mol of the conformation to the most stable conformation, R is the molar ideal gas constant which has value of 8.31 J/(mol•K), and T is temperature in kelvins (K).

Molecular structure was first optimized. Then the dihedral angle between porphyrin plane and imide porphyrin was changed to make new input files of every 5° in range of 5˚-90˚. The molecular energy was calculated without further optimizing the molecular structure. Relative energy is the energy relative to most stable structure (which has dihedral angle of 90˚). Probability was calculated using Boltzmann Distribution at 298 K and normalized by dividing the total probability. Since the molecule structures with dihedral angle 95˚-175˚ used same energy and probability as that with the of 85˚-5˚ since they are symmetric.

Result was seen in figure 7 showing that at 298 K, the dihedral angel would have 80% to be from 80˚ to 100˚, and more than 94% probability to be from 75˚ to 105˚.

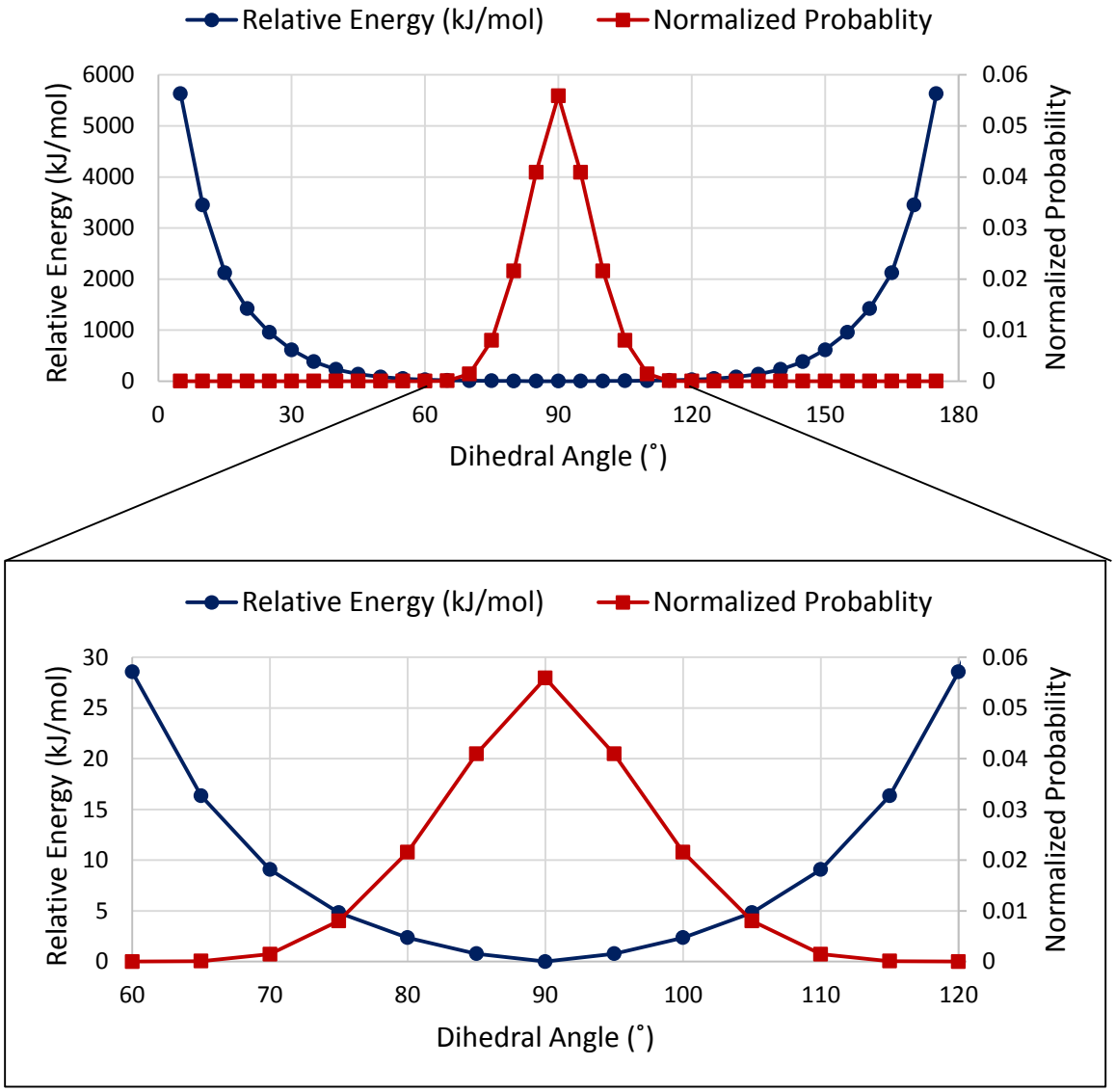


Figure S12. Dihedral angle dependence of relative energy porphyrin-imide molecule

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2. I. Rungger and S. Sanvito, Phys. Rev. B. **78**, 035407 (2008).

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4. J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon and D. Sanchez-Portal, J. Phys.: Condens. Matter **14**, 2745-2779 (2002).

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9. R. Yamada, K. Albrecht, T. Ohto, K. Minode, K. Yamamoto and H. Tada, Nanoscale, **10**, 19818-19824 (2018).
10. M. L. Perrin, M. Doelman, R. Eelkema, and H. S. J. van der Zant, Phys. Chem. Chem. Phys., **19**, 29187-29194 2017.

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PeriodicTransp              T       #mx periodic calculation or not
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Smeagol-trans!!!!)
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Input file for Rh

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PAO.EnergyShift             20 meV

%block PAO.BasisSizes
H      DZP
C      DZP
O      DZP
N      DZP
Au     SZP
Rh     DZP
I      DZP
%endblock PAO.BasisSizes
MeshCutoff                  300. Ry             # Mesh cutoff. real space mesh
# Kpoints
%block kgrid_Monkhorst_Pack
     2       0       0         0
     0       2       0         0
```

```
    0       0       1         0
%endblock kgrid_Monkhorst_Pack
# Function
xc.functional              GGA               # Exchange-correlation functional
xc.authors                  PBE              # Exchange-correlation version
SpinPolarized               .true.         # Logical parameters are: yes or no
# SCF options
MaxSCFIterations          1000              # Maximum number of SCF iter
DM.MixingWeight            0.001                # New DM amount for next SCF cycle
DM.Tolerance               1.d-4             # Tolerance in maximum difference
                                               # between input and output DM
#DM.UseSaveDM                true                # to use continuation files
DM.NumberPulay               5
SolutionMethod              diagon           # OrderN or Diagon
OccupationFunction        FD                  # FD or MP
ElectronicTemperature    200 K            # Temp. for Fermi smearing
# MD options
MD.TypeOfRun                 cg                # Type of dynamics:
MD.NumCGsteps                  0               # Number of CG steps for
                                              #      coordinate optimization
MD.MaxCGDispl                0.2 Ang        # Maximum atomic displacement
                                              #      in one CG step (Bohr)
MD.MaxForceTol             0.04 eV/Ang    # Tolerance in the maximum
                                              #      atomic force (Ry/Bohr)
MD.VariableCell             .false.
# ============================================================
##For Smeagol-trans
InitTransport      F        #reset "nsc process" as siesta or not,'true' as siesta
EMTransport                    T         #NEGF method or not
NSlices                          1       # the number of layers for x in mx
PeriodicTransp                T         #mx periodic calculation or not
NEnergReal                      0          # E-points for NE
NEnergImCircle                16         # E-points for EQ-Circle
NEnergImLine                   16          # E-points for EQ-Line
NPoles                           16          # E-points for EQ-Pole
Delta                            1.d-4
EnergLowestBound           -6.0d0    Ry      # Absolute value
```

```
#Bias Setup
VInitial                        0.0 eV
VFinal                          0.0 eV
NIVPoints                       0
%block SaveBiasSteps
   0
%endblock SaveBiasSteps
#Fock shift Control(!!!!Vary Every Time while Smeagol-trans!!!!)
HartreeLeadsBottom          -19.62229156      eV       # Matlab: VHplot('0.lead.VH')
HartreeLeadsLeft              0.000    Ang              #The mx's atomic z-coordinates of the
corresponding 'HartreeLeadsBottom' position at left
HartreeLeadsRight             0.000    Ang       # The mx's atomic z-coordinates of the
corresponding 'HartreeLeadsBottom' position at right
##Transport Output Flags
TrCoefficients                T       #generate '*.TRC' file or not
TransmissionOverk             T       #generate '*.TRC.k.up/down' file,containning infor about T(E,k)
NTransmPoints                 512
TRCScaleEf       T
InitTransmRange            -4.0 eV       #(!!!!Vary Every Time with respect to lead's Ef while
Smeagol-trans!!!!)
FinalTransmRange            4.0 eV
SaveElectrostaticPotential       T
SaveRHO       T
#Sensible parameters for structural change
FullRamp     T
MixHamiltonian         T # F
ReadHamiltonian       T # F
DM.MixSCF1              T # F
DM.UseSaveDM     T
#Force Options
EM.CalculateForces                  T
EM.SetEBD    T
WriteForces          T
WriteCoorXmol        T     # Write Atoms coordinates
WriteEigenvalues                    F
Sigma.SVDTolZero    1.0d-7
EM.Timings T
```

```
Sigma.WriteToDisk                    F         # Default value
WriteCoorStep      T
# Structure
LatticeConstant    1.000 Ang

%block LatticeVectors
    14.42497835       0.00000000       0.00000000
     7.21248915      12.49239770       0.00000000
     0.00000000       0.00000000      63.95264230
%endblock LatticeVectors

# Atomic coordinates
AtomicCoordinatesFormat         Ang
%block AtomicCoordinatesAndAtomicSpecies
    1.44249783      0.83282651      0.00000000 5 #    Au 1
    4.32749350      0.83282651      0.00000000 5 #    Au 2
    7.21248917      0.83282651      0.00000000 5 #    Au 3
   10.09748484      0.83282651      0.00000000 5 #    Au 4
   12.98248051      0.83282651      0.00000000 5 #    Au 5
    2.88499566      3.33130605      0.00000000 5 #    Au 6
    5.76999133      3.33130605      0.00000000 5 #    Au 7
    8.65498700      3.33130605      0.00000000 5 #    Au 8
   11.53998267      3.33130605      0.00000000 5 #    Au 9
   14.42497834      3.33130605      0.00000000 5 #    Au 10
    4.32749349      5.82978559      0.00000000 5 #    Au 11
    7.21248916      5.82978559      0.00000000 5 #    Au 12
   10.09748483      5.82978559      0.00000000 5 #    Au 13
   12.98248050      5.82978559      0.00000000 5 #    Au 14
   15.86747617      5.82978559      0.00000000 5 #    Au 15
    5.76999132      8.32826513      0.00000000 5 #    Au 16
    8.65498699      8.32826513      0.00000000 5 #    Au 17
   11.53998266      8.32826513      0.00000000 5 #    Au 18
   14.42497833      8.32826513      0.00000000 5 #    Au 19
   17.30997400      8.32826513      0.00000000 5 #    Au 20
    7.21248915     10.82674467      0.00000000 5 #    Au 21
   10.09748482     10.82674467      0.00000000 5 #    Au 22
   12.98248049     10.82674467      0.00000000 5 #    Au 23
```

15.86747616	10.82674467	0.00000000	5 #	Au 24
18.75247183	10.82674467	0.00000000	5 #	Au 25
0.00000000	0.00000000	2.35558910	5 #	Au 26
2.88499567	0.00000000	2.35558910	5 #	Au 27
5.76999134	0.00000000	2.35558910	5 #	Au 28
8.65498701	0.00000000	2.35558910	5 #	Au 29
11.53998268	0.00000000	2.35558910	5 #	Au 30
1.44249783	2.49847954	2.35558910	5 #	Au 31
4.32749350	2.49847954	2.35558910	5 #	Au 32
7.21248917	2.49847954	2.35558910	5 #	Au 33
10.09748484	2.49847954	2.35558910	5 #	Au 34
12.98248051	2.49847954	2.35558910	5 #	Au 35
2.88499566	4.99695908	2.35558910	5 #	Au 36
5.76999133	4.99695908	2.35558910	5 #	Au 37
8.65498700	4.99695908	2.35558910	5 #	Au 38
11.53998267	4.99695908	2.35558910	5 #	Au 39
14.42497834	4.99695908	2.35558910	5 #	Au 40
4.32749349	7.49543862	2.35558910	5 #	Au 41
7.21248916	7.49543862	2.35558910	5 #	Au 42
10.09748483	7.49543862	2.35558910	5 #	Au 43
12.98248050	7.49543862	2.35558910	5 #	Au 44
15.86747617	7.49543862	2.35558910	5 #	Au 45
5.76999132	9.99391816	2.35558910	5 #	Au 46
8.65498699	9.99391816	2.35558910	5 #	Au 47
11.53998266	9.99391816	2.35558910	5 #	Au 48
14.42497833	9.99391816	2.35558910	5 #	Au 49
17.30997400	9.99391816	2.35558910	5 #	Au 50
2.88499567	1.66565303	4.71117820	5 #	Au 51
5.76999134	1.66565303	4.71117820	5 #	Au 52
8.65498701	1.66565303	4.71117820	5 #	Au 53
11.53998268	1.66565303	4.71117820	5 #	Au 54
14.42497835	1.66565303	4.71117820	5 #	Au 55
4.32749350	4.16413257	4.71117820	5 #	Au 56
7.21248917	4.16413257	4.71117820	5 #	Au 57
10.09748484	4.16413257	4.71117820	5 #	Au 58
12.98248051	4.16413257	4.71117820	5 #	Au 59
15.86747618	4.16413257	4.71117820	5 #	Au 60

5.76999133	6.66261211	4.71117820	5 #	Au 61
8.65498700	6.66261211	4.71117820	5 #	Au 62
11.53998267	6.66261211	4.71117820	5 #	Au 63
14.42497834	6.66261211	4.71117820	5 #	Au 64
17.30997401	6.66261211	4.71117820	5 #	Au 65
7.21248916	9.16109165	4.71117820	5 #	Au 66
10.09748483	9.16109165	4.71117820	5 #	Au 67
12.98248050	9.16109165	4.71117820	5 #	Au 68
15.86747617	9.16109165	4.71117820	5 #	Au 69
18.75247184	9.16109165	4.71117820	5 #	Au 70
8.65498699	11.65957119	4.71117820	5 #	Au 71
11.53998266	11.65957119	4.71117820	5 #	Au 72
14.42497833	11.65957119	4.71117820	5 #	Au 73
17.30997400	11.65957119	4.71117820	5 #	Au 74
20.19496967	11.65957119	4.71117820	5 #	Au 75
1.44249783	0.83282651	7.06676730	5 #	Au 76
4.32749350	0.83282651	7.06676730	5 #	Au 77
7.21248917	0.83282651	7.06676730	5 #	Au 78
10.09748484	0.83282651	7.06676730	5 #	Au 79
12.98248051	0.83282651	7.06676730	5 #	Au 80
2.88499566	3.33130605	7.06676730	5 #	Au 81
5.76999133	3.33130605	7.06676730	5 #	Au 82
8.65498700	3.33130605	7.06676730	5 #	Au 83
11.53998267	3.33130605	7.06676730	5 #	Au 84
14.42497834	3.33130605	7.06676730	5 #	Au 85
4.32749349	5.82978559	7.06676730	5 #	Au 86
7.21248916	5.82978559	7.06676730	5 #	Au 87
10.09748483	5.82978559	7.06676730	5 #	Au 88
12.98248050	5.82978559	7.06676730	5 #	Au 89
15.86747617	5.82978559	7.06676730	5 #	Au 90
5.76999132	8.32826513	7.06676730	5 #	Au 91
8.65498699	8.32826513	7.06676730	5 #	Au 92
11.53998266	8.32826513	7.06676730	5 #	Au 93
14.42497833	8.32826513	7.06676730	5 #	Au 94
17.30997400	8.32826513	7.06676730	5 #	Au 95
7.21248915	10.82674467	7.06676730	5 #	Au 96
10.09748482	10.82674467	7.06676730	5 #	Au 97

12.98248049	10.82674467	7.06676730	5 #	Au 98
15.86747616	10.82674467	7.06676730	5 #	Au 99
18.75247183	10.82674467	7.06676730	5 #	Au 100
0.00000000	0.00000000	9.42235639	5 #	Au 101
2.88499567	0.00000000	9.42235639	5 #	Au 102
5.76999134	0.00000000	9.42235639	5 #	Au 103
8.65498701	0.00000000	9.42235639	5 #	Au 104
11.53998268	0.00000000	9.42235639	5 #	Au 105
1.44249783	2.49847954	9.42235639	5 #	Au 106
4.32749350	2.49847954	9.42235639	5 #	Au 107
7.21248917	2.49847954	9.42235639	5 #	Au 108
10.09748484	2.49847954	9.42235639	5 #	Au 109
12.98248051	2.49847954	9.42235639	5 #	Au 110
2.88499566	4.99695908	9.42235639	5 #	Au 111
5.76999133	4.99695908	9.42235639	5 #	Au 112
8.65498700	4.99695908	9.42235639	5 #	Au 113
11.53998267	4.99695908	9.42235639	5 #	Au 114
14.42497834	4.99695908	9.42235639	5 #	Au 115
4.32749349	7.49543862	9.42235639	5 #	Au 116
7.21248916	7.49543862	9.42235639	5 #	Au 117
10.09748483	7.49543862	9.42235639	5 #	Au 118
12.98248050	7.49543862	9.42235639	5 #	Au 119
15.86747617	7.49543862	9.42235639	5 #	Au 120
5.76999132	9.99391816	9.42235639	5 #	Au 121
8.65498699	9.99391816	9.42235639	5 #	Au 122
11.53998266	9.99391816	9.42235639	5 #	Au 123
14.42497833	9.99391816	9.42235639	5 #	Au 124
17.30997400	9.99391816	9.42235639	5 #	Au 125
2.93221647	1.69652329	11.78248994	5 #	Au 126
11.49672213	1.69705280	11.78511097	5 #	Au 127
14.42553831	2.03738142	11.81326275	5 #	Au 128
7.21347822	9.14006547	11.80407995	5 #	Au 129
8.90856911	11.52125528	11.81853683	5 #	Au 130
19.94878592	11.52639788	11.81750636	5 #	Au 131
1.46885775	0.89149655	13.97927220	5 #	Au 132
12.96076452	0.89508396	13.98461598	5 #	Au 133
7.21418537	10.79580913	14.02856624	5 #	Au 134

-0.02507590 -0.11763859 15.93322599 3 # O 135
-0.04918644 -0.12450299 17.27143147 2 # C 136
-0.03787238 2.05828742 17.44961509 1 # H 137
-0.06327970 -2.30469054 17.47175368 1 # H 138
-0.06878258 -1.34491370 18.02720884 2 # C 139
-0.05502218 1.10594722 18.01585910 2 # C 140
-0.09591600 -1.33541939 19.42739445 2 # C 141
-0.08231926 1.11262586 19.41478178 2 # C 142
-0.11240853 -2.29547355 19.97832526 1 # H 143
-0.08671641 2.07951061 19.95389635 1 # H 144
-0.10572389 -0.10787150 20.16892037 2 # C 145
-0.14067210 -0.10122657 21.60301366 2 # C 146
-0.17267877 -0.09838185 22.85244525 2 # C 147
-0.13893008 -2.79492810 23.22343959 1 # H 148
-0.22902455 2.60062269 23.22733279 1 # H 149
-0.17359366 -2.64972357 24.31574795 2 # C 150
-0.24046878 2.45358019 24.31981569 2 # C 151
-0.20004880 -0.09803962 24.28615975 2 # C 152
-0.19780996 -1.35587372 24.97312747 2 # C 153
-0.22505268 1.15864940 24.97495273 2 # C 154
-0.18190182 -4.70441424 25.20402992 1 # H 155
-0.28003163 4.50625168 25.21157150 1 # H 156
-0.19536853 -3.60586433 25.31021861 2 # C 157
-0.26613512 3.40763470 25.31631506 2 # C 158
-0.21165114 -1.52133570 26.35131070 4 # N 159
-0.22475259 1.32174670 26.35351098 4 # N 160
-0.22808209 -2.89491901 26.57486572 2 # C 161
-0.26334283 2.69430404 26.58003788 2 # C 162
-2.95195032 -0.10653860 27.82391842 7 # I 163
-0.27513579 -4.62637172 27.83401651 1 # H 164
-0.25840357 -3.51931630 27.83442228 2 # C 165
-0.32130234 -0.10172469 27.83503929 6 # Rh 166
-0.27682668 3.31601501 27.84144245 2 # C 167
-0.30336507 4.42293972 27.84366764 1 # H 168
-0.25917831 -2.89451605 29.09551856 2 # C 169
-0.25153154 2.68849654 29.10107607 2 # C 170
-0.22896915 -1.52439091 29.31657780 4 # N 171

-0.22366086 1.31777027 29.31909521 4 # N 172
-0.26490659 -3.60518316 30.36251074 2 # C 173
-0.23649883 3.39602384 30.36985727 2 # C 174
-0.27209729 -4.70363077 30.47039215 1 # H 175
-0.23471275 4.49407274 30.48073359 1 # H 176
-0.23721381 -1.35604073 30.69864692 2 # C 177
-0.22096397 1.14603428 30.70100345 2 # C 178
-0.22298748 -0.10580849 31.36071399 2 # C 179
-0.24903100 -2.65097521 31.35763933 2 # C 180
-0.21379914 2.43945817 31.36258729 2 # C 181
-0.24295997 -2.81138684 32.44816432 1 # H 182
-0.19141290 2.59747724 32.45321412 1 # H 183
2.11583067 -0.12161451 32.79126631 3 # O 184
-0.20271134 -0.10832980 32.81902376 4 # N 185
-2.52072899 -0.08726955 32.87229422 3 # O 186
1.07499345 -0.11764913 33.45704326 2 # C 187
-1.45903094 -0.09801514 33.50106363 2 # C 188
1.07544261 -0.12141397 34.96235845 2 # C 189
-1.40711577 -0.10063455 35.00570817 2 # C 190
3.23417661 -0.13836781 35.07325265 1 # H 191
-3.56063472 -0.08032589 35.18987961 1 # H 192
2.29514637 -0.13192466 35.66078772 2 # C 193
-0.15371203 -0.11241651 35.69039458 2 # C 194
-2.60239616 -0.09036614 35.74537742 2 # C 195
2.31846680 -0.13386530 37.08148958 2 # C 196
-0.12914333 -0.11486102 37.13123713 2 # C 197
-2.57734032 -0.09290462 37.16593914 2 # C 198
3.27564952 -0.14100195 37.63922718 1 # H 199
-3.51504996 -0.08464916 37.75598311 1 # H 200
1.12230906 -0.12529620 37.81899228 2 # C 201
-1.35628830 -0.10527790 37.86141664 2 # C 202
1.17089752 -0.12266495 39.32672595 2 # C 203
-1.35264913 -0.10458125 39.36958975 2 # C 204
2.23978497 -0.12847791 39.94716422 3 # O 205
-0.07946178 -0.11256327 40.01116109 4 # N 206
-2.39958512 -0.09680562 40.02624773 3 # O 207
-0.05695958 -0.09208073 41.47167182 2 # C 208

-0.04063581	2.08752168	41.60234803	1 #	H 209
-0.06815480	-2.26736049	41.67461341	1 #	H 210
-0.04131049	1.13685538	42.17039096	2 #	C 211
-0.05679740	-1.29785084	42.21061574	2 #	C 212
-0.02822381	1.16277782	43.57807368	2 #	C 213
-0.04381012	-1.27641642	43.61790984	2 #	C 214
-0.01620861	2.13110874	44.11703391	1 #	H 215
-0.04409780	-2.22716018	44.18730333	1 #	H 216
-0.03138365	-0.04406353	44.34124035	2 #	C 217
-0.02107128	-0.02329816	45.70277841	3 #	O 218
14.42682790	1.68681409	47.56586444	5 #	Au 219
8.70076526	11.61272683	47.58407929	5 #	Au 220
20.14966743	11.60843876	47.57983078	5 #	Au 221
1.68896600	0.96381117	49.77591271	5 #	Au 222
12.74204225	0.95951264	49.77636373	5 #	Au 223
14.42547056	3.35116208	49.79093885	5 #	Au 224
7.21244729	10.53751623	49.78442844	5 #	Au 225
10.14208804	10.80070641	49.80254040	5 #	Au 226
18.70951844	10.80034766	49.80058023	5 #	Au 227
0.00000000	0.00000000	52.17469681	5 #	Au 228
2.88499572	0.00000000	52.17469681	5 #	Au 229
5.76999145	0.00000000	52.17469681	5 #	Au 230
8.65498717	0.00000000	52.17469681	5 #	Au 231
11.53998290	0.00000000	52.17469681	5 #	Au 232
1.44249786	2.49847959	52.17469681	5 #	Au 233
4.32749358	2.49847959	52.17469681	5 #	Au 234
7.21248931	2.49847959	52.17469681	5 #	Au 235
10.09748503	2.49847959	52.17469681	5 #	Au 236
12.98248076	2.49847959	52.17469681	5 #	Au 237
2.88499571	4.99695918	52.17469681	5 #	Au 238
5.76999144	4.99695918	52.17469681	5 #	Au 239
8.65498716	4.99695918	52.17469681	5 #	Au 240
11.53998289	4.99695918	52.17469681	5 #	Au 241
14.42497861	4.99695918	52.17469681	5 #	Au 242
4.32749357	7.49543876	52.17469681	5 #	Au 243
7.21248930	7.49543876	52.17469681	5 #	Au 244
10.09748502	7.49543876	52.17469681	5 #	Au 245

12.98248075	7.49543876	52.17469681	5 #	Au 246
15.86747647	7.49543876	52.17469681	5 #	Au 247
5.76999143	9.99391835	52.17469681	5 #	Au 248
8.65498715	9.99391835	52.17469681	5 #	Au 249
11.53998288	9.99391835	52.17469681	5 #	Au 250
14.42497860	9.99391835	52.17469681	5 #	Au 251
17.30997433	9.99391835	52.17469681	5 #	Au 252
2.88499572	1.66565306	54.53028596	5 #	Au 253
5.76999145	1.66565306	54.53028596	5 #	Au 254
8.65498717	1.66565306	54.53028596	5 #	Au 255
11.53998290	1.66565306	54.53028596	5 #	Au 256
14.42497862	1.66565306	54.53028596	5 #	Au 257
4.32749358	4.16413265	54.53028596	5 #	Au 258
7.21248931	4.16413265	54.53028596	5 #	Au 259
10.09748503	4.16413265	54.53028596	5 #	Au 260
12.98248076	4.16413265	54.53028596	5 #	Au 261
15.86747648	4.16413265	54.53028596	5 #	Au 262
5.76999144	6.66261224	54.53028596	5 #	Au 263
8.65498716	6.66261224	54.53028596	5 #	Au 264
11.53998289	6.66261224	54.53028596	5 #	Au 265
14.42497861	6.66261224	54.53028596	5 #	Au 266
17.30997434	6.66261224	54.53028596	5 #	Au 267
7.21248930	9.16109182	54.53028596	5 #	Au 268
10.09748502	9.16109182	54.53028596	5 #	Au 269
12.98248075	9.16109182	54.53028596	5 #	Au 270
15.86747647	9.16109182	54.53028596	5 #	Au 271
18.75247220	9.16109182	54.53028596	5 #	Au 272
8.65498715	11.65957141	54.53028596	5 #	Au 273
11.53998288	11.65957141	54.53028596	5 #	Au 274
14.42497860	11.65957141	54.53028596	5 #	Au 275
17.30997433	11.65957141	54.53028596	5 #	Au 276
20.19497005	11.65957141	54.53028596	5 #	Au 277
1.44249783	0.83282651	56.88587501	5 #	Au 278
4.32749350	0.83282651	56.88587501	5 #	Au 279
7.21248917	0.83282651	56.88587501	5 #	Au 280
10.09748484	0.83282651	56.88587501	5 #	Au 281
12.98248051	0.83282651	56.88587501	5 #	Au 282

2.88499566	3.33130605	56.88587501	5 #	Au 283
5.76999133	3.33130605	56.88587501	5 #	Au 284
8.65498700	3.33130605	56.88587501	5 #	Au 285
11.53998267	3.33130605	56.88587501	5 #	Au 286
14.42497834	3.33130605	56.88587501	5 #	Au 287
4.32749349	5.82978559	56.88587501	5 #	Au 288
7.21248916	5.82978559	56.88587501	5 #	Au 289
10.09748483	5.82978559	56.88587501	5 #	Au 290
12.98248050	5.82978559	56.88587501	5 #	Au 291
15.86747617	5.82978559	56.88587501	5 #	Au 292
5.76999132	8.32826513	56.88587501	5 #	Au 293
8.65498699	8.32826513	56.88587501	5 #	Au 294
11.53998266	8.32826513	56.88587501	5 #	Au 295
14.42497833	8.32826513	56.88587501	5 #	Au 296
17.30997400	8.32826513	56.88587501	5 #	Au 297
7.21248915	10.82674467	56.88587501	5 #	Au 298
10.09748482	10.82674467	56.88587501	5 #	Au 299
12.98248049	10.82674467	56.88587501	5 #	Au 300
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12.98248051	2.49847954	59.24146410	5 #	Au 312
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8.65498700	4.99695908	59.24146410	5 #	Au 315
11.53998267	4.99695908	59.24146410	5 #	Au 316
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7.21248916	7.49543862	59.24146410	5 #	Au 319

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  5.76999132    9.99391816   59.24146410 5 #   Au 323
  8.65498699    9.99391816   59.24146410 5 #   Au 324
 11.53998266    9.99391816   59.24146410 5 #   Au 325
 14.42497833    9.99391816   59.24146410 5 #   Au 326
 17.30997400    9.99391816   59.24146410 5 #   Au 327
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 11.53998268    1.66565303   61.59705320 5 #   Au 331
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 12.98248051    4.16413257   61.59705320 5 #   Au 336
 15.86747618    4.16413257   61.59705320 5 #   Au 337
  5.76999133    6.66261211   61.59705320 5 #   Au 338
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 17.30997401    6.66261211   61.59705320 5 #   Au 342
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 10.09748483    9.16109165   61.59705320 5 #   Au 344
 12.98248050    9.16109165   61.59705320 5 #   Au 345
 15.86747617    9.16109165   61.59705320 5 #   Au 346
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 11.53998266   11.65957119   61.59705320 5 #   Au 349
 14.42497833   11.65957119   61.59705320 5 #   Au 350
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