

Supporting Information

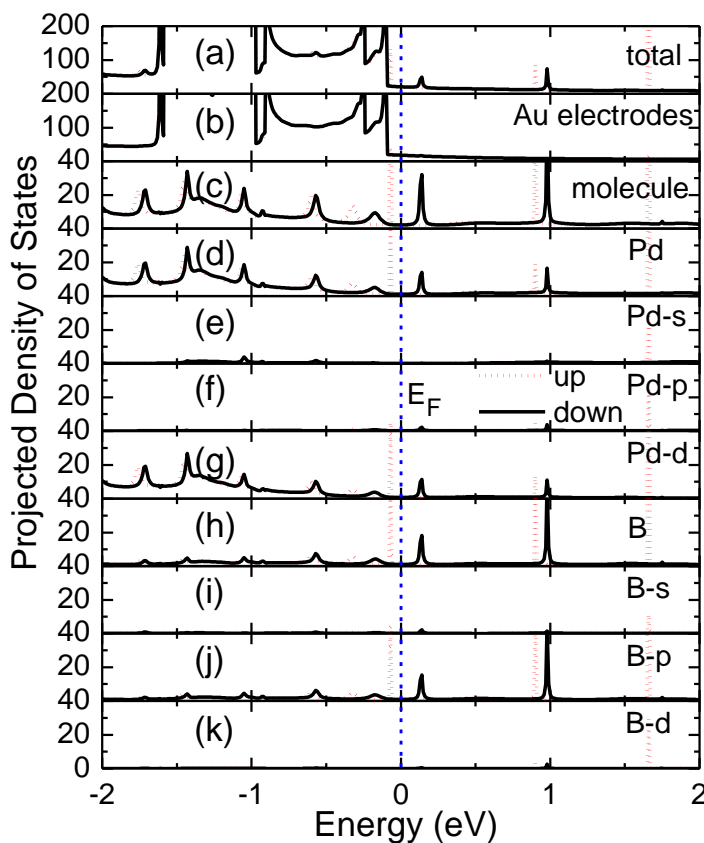


Figure S1. (a)-(k) The PDOS analysis of the two-probe system shown in Fig. 1(d) under 20% tensile strain along A, A120Bfree, corresponding to the transmission spectra in Fig. 5(d).

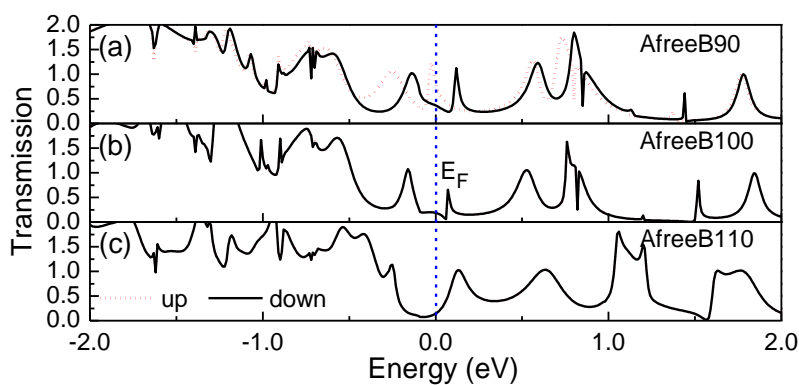


Figure S2. (a)-(c) Transmission spectra of Pd₉B₁₆ contacted with atomic Au chain electrodes, under different strains along B.

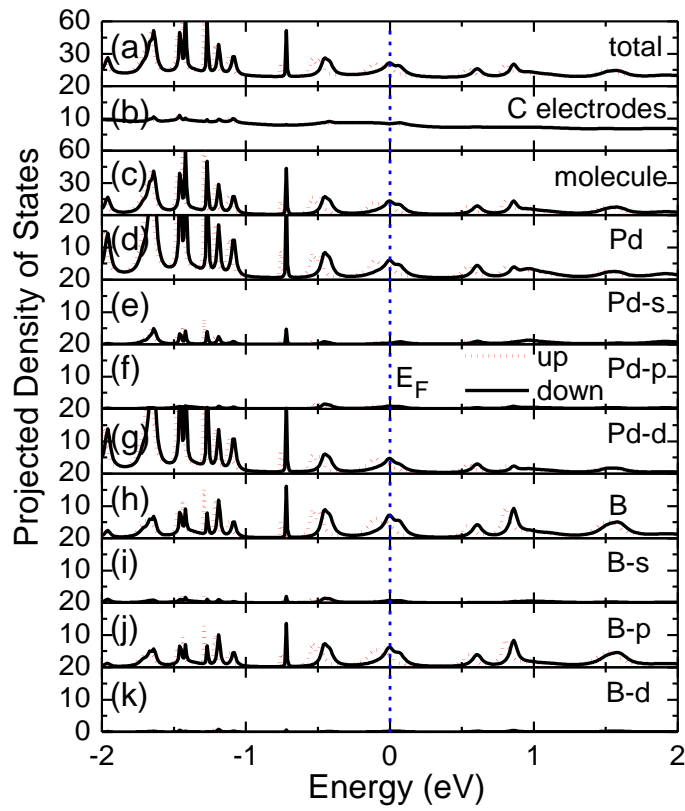


Figure S3. (a)-(k) The PDOS analysis of the two-probe system shown in Fig. 1(e) under 10% tensile strain along A, A110Bfree, corresponding to the transmission spectra in Fig. 6(c).

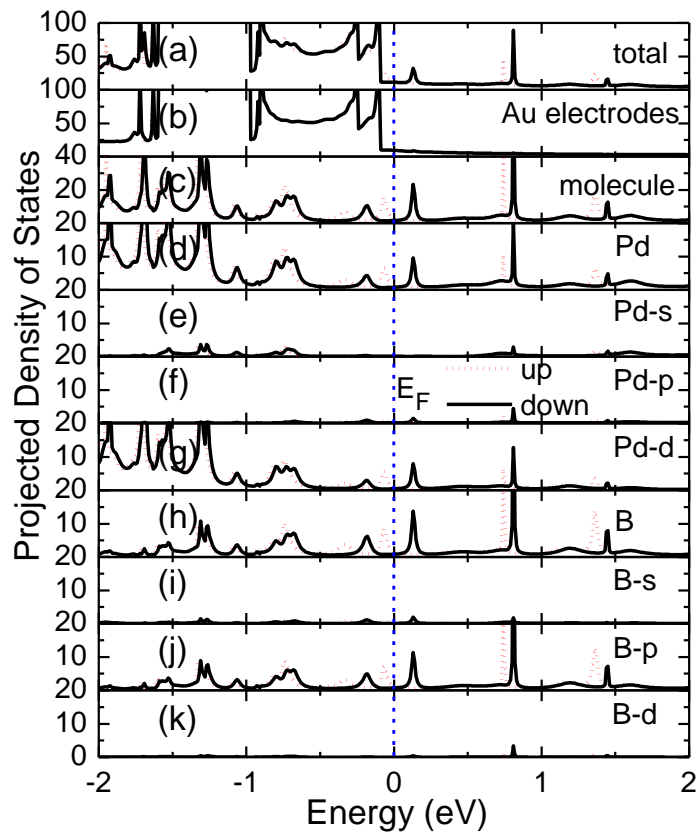


Figure S4. (a)-(k) The PDOS analysis of AuL1-A100Bfree-AuR2 system, where is no strain applied, corresponding to the transmission spectra in Fig. 8(b).

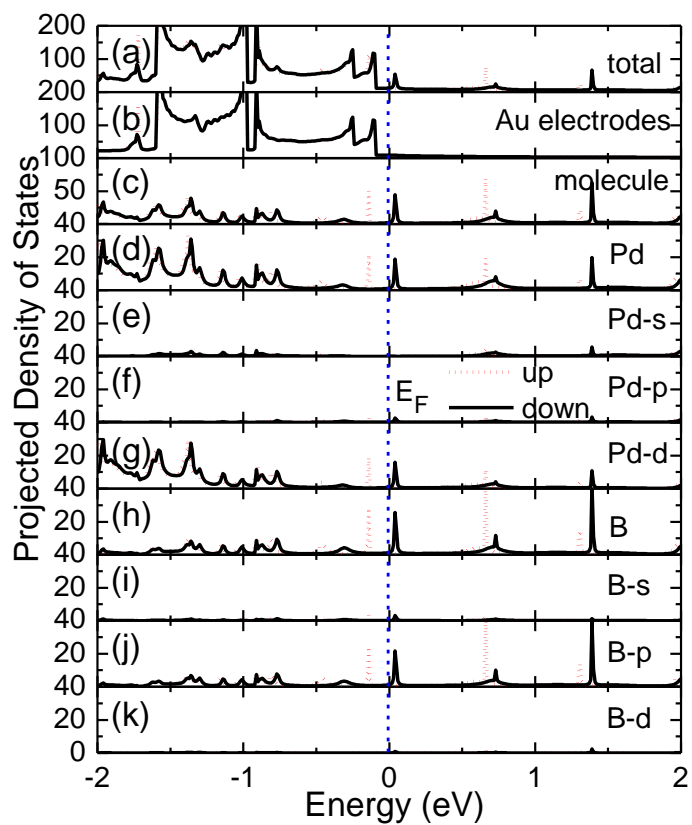


Figure S5. (a)-(k) The PDOS analysis of AuL1-A100Bfree-AuR3 system, where is no strain applied, corresponding to the transmission spectra in Fig. 8(c).

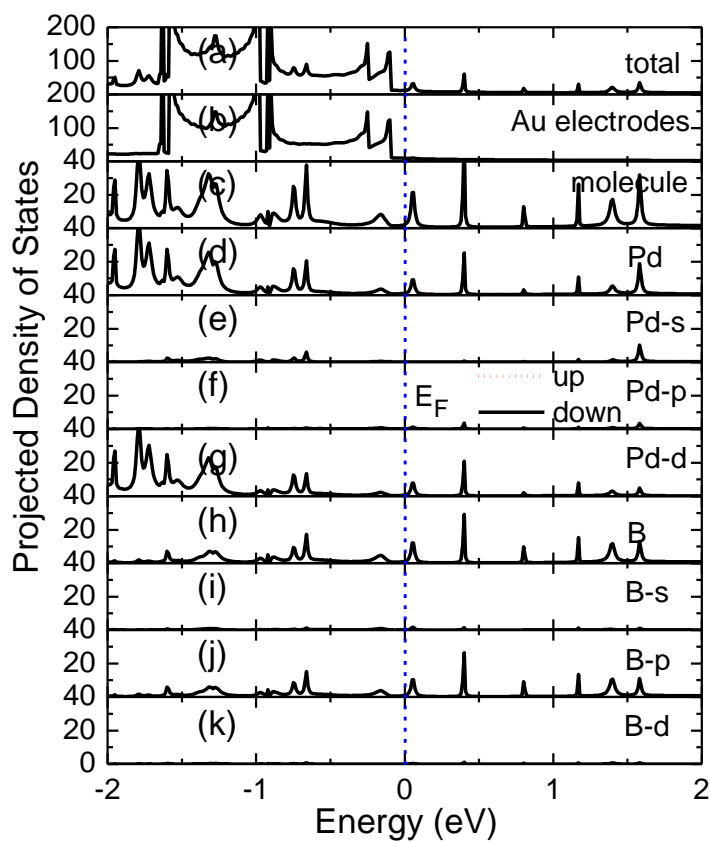


Figure S6. (a)-(k) The PDOS analysis of AuL2-A100Bfree-AuR2 system, where is no strain applied, corresponding to the transmission spectra in Fig. 8(d).

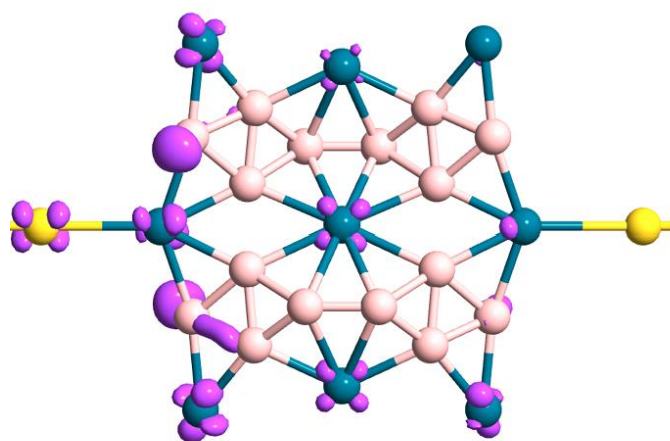


Figure S7. The local device density of states for AuL2-A100Bfree-AuR2 system contacted with atomic Au chain electrodes.

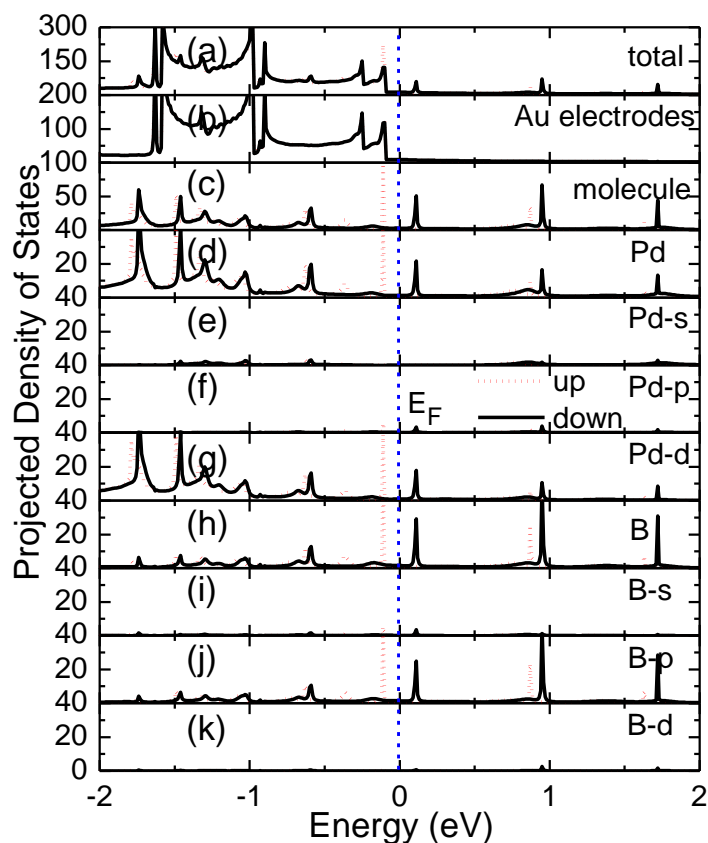


Figure S8. (a)-(k) The PDOS analysis of AuL1-A120Bfree-AuR3 system under 20% tensile strain along A, corresponding to the transmission spectra in Fig. 9(c).

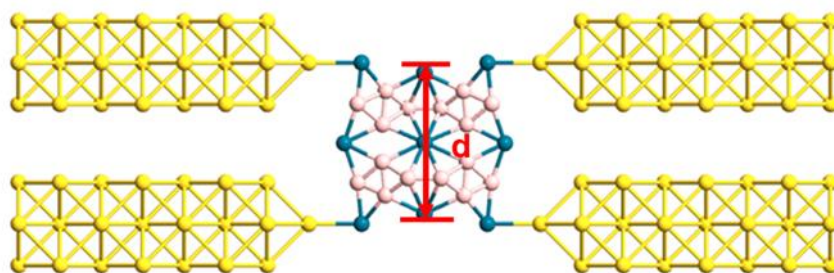


Fig. S9. The illustration of two-probe A100Bfree system.

Table S1. The lateral widths (denoted by d in Fig. S9) and variations for A100Bfree and A100Bfree systems under non dispersion correction, Grimme DFT-D2 and Grimme DFT-D3 methods, respectively.

Configuration	vdW	d (Å)	Δd	$\Delta d/d$
A100Bfree	non	6.92		

	DFT-D2	6.88	-0.04	-0.58%
	DFT-D3	6.95	0.03	0.43%
A110Bfree	non	7.08		
	DFT-D2	6.99	-0.09	-1.27%
	DFT-D3	7.10	0.02	0.28%

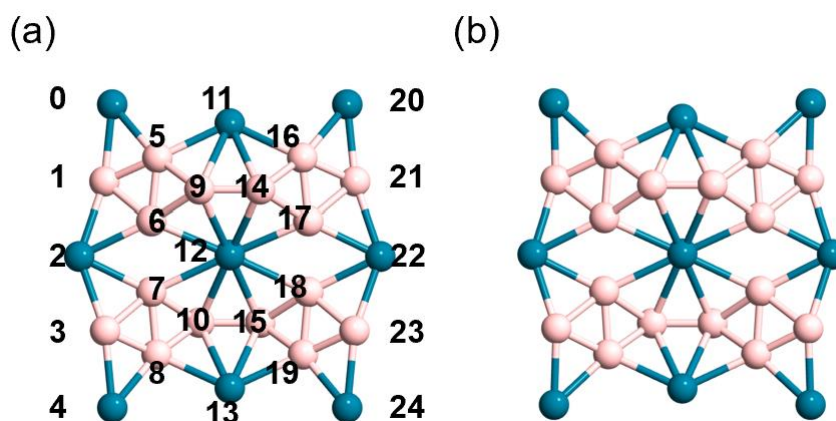


Figure S10. (a) A100Bfree (b) A110Bfree molecule.

Table S2. The bond lengths in A100Bfree and A110Bfree molecules.

Bond	Bond length of A100Bfree (Å)	Bond length of A110Bfree (Å)
B ₀₋₁	2.04066	2.01452
B ₁₋₂	2.10278	2.08748
B ₅₋₆	1.65104	1.66828
B ₉₋₁₁	2.27152	2.2379
B ₉₋₁₂	2.24448	2.24292
B ₀₋₅	2.03212	2.06125
B ₁₋₅	1.66624	1.66582
B ₁₋₆	1.7425	1.73284
B ₂₋₆	2.11244	2.12576
B ₅₋₁₁	2.12287	2.15794
B ₅₋₉	1.66912	1.675
B ₆₋₉	1.74882	1.7573
B ₆₋₁₂	2.25994	2.26797
B ₂₋₃	2.10451	2.08918
B ₃₋₄	2.0407	2.01682
B ₇₋₈	1.6502	1.66682
B ₁₀₋₁₂	2.23896	2.23983
B ₁₀₋₁₃	2.26188	2.23136
B ₂₋₇	2.1183	2.13145

B ₃₋₇	1.73318	1.72352
B ₃₋₈	1.65768	1.65928
B ₄₋₈	2.0376	2.06404
B ₇₋₁₂	2.28256	2.28451
B ₇₋₁₀	1.75954	1.76078
B ₈₋₁₀	1.65986	1.66468
B ₈₋₁₃	2.13967	2.17248
B ₉₋₁₄	1.60782	1.59198
B ₁₀₋₁₅	1.5919	1.59469
B ₁₁₋₁₄	2.27849	2.23791
B ₁₂₋₁₄	2.24452	2.24292
B ₁₆₋₁₇	1.65104	1.66827
B ₂₀₋₂₁	2.04066	2.01453
B ₂₁₋₂₂	2.10278	2.08748
B ₁₁₋₁₆	2.14051	2.15796
B ₁₄₋₁₆	1.66913	1.67499
B ₁₄₋₁₇	1.76289	1.7573
B ₁₂₋₁₇	2.25999	2.26797
B ₁₆₋₂₀	2.03214	2.06125
B ₁₆₋₂₁	1.66623	1.66582
B ₁₇₋₂₁	1.74975	1.73283
B ₁₇₋₂₂	2.11242	2.12576
B ₁₂₋₁₅	2.23898	2.23983
B ₁₃₋₁₅	2.26191	2.23135
B ₁₈₋₁₉	1.6502	1.66682
B ₂₂₋₂₃	2.10455	2.08917
B ₂₃₋₂₄	2.04075	2.01682
B ₁₂₋₁₈	2.28258	2.28451
B ₁₅₋₁₈	1.75953	1.76076
B ₁₅₋₁₉	1.65987	1.66468
B ₁₃₋₁₉	2.13976	2.17243
B ₁₈₋₂₂	2.11825	2.13145
B ₁₈₋₂₃	1.73322	1.72352
B ₁₉₋₂₃	1.65766	1.67138
B ₁₉₋₂₄	2.03768	2.06406

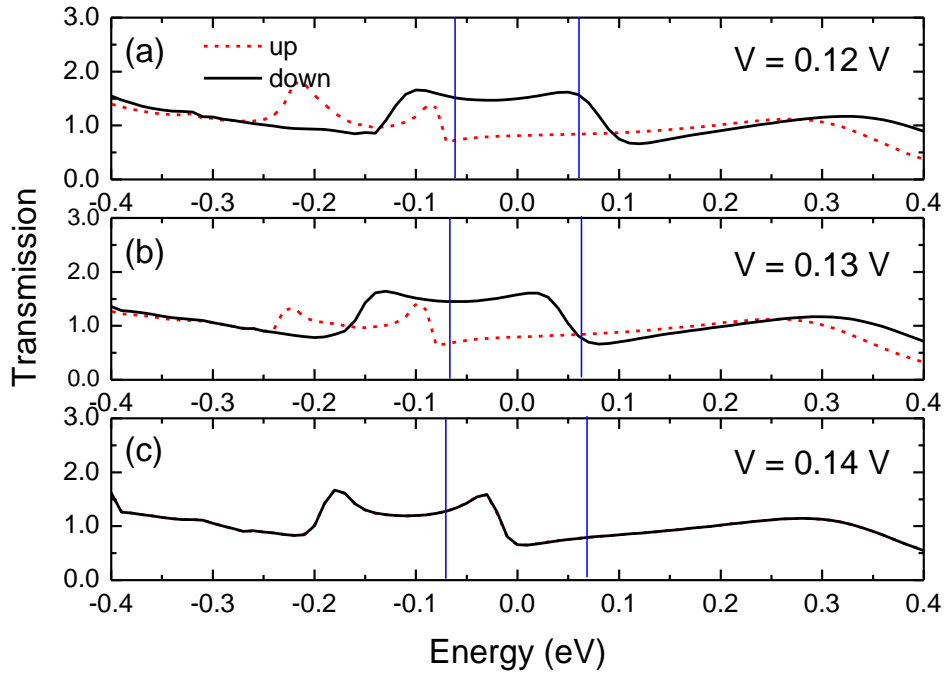


Fig. S11. (a)-(c) The transmission spectra for the two-probe system of A130Bfree under the biases of 0.12, 0.13 and 0.14 V, respectively.

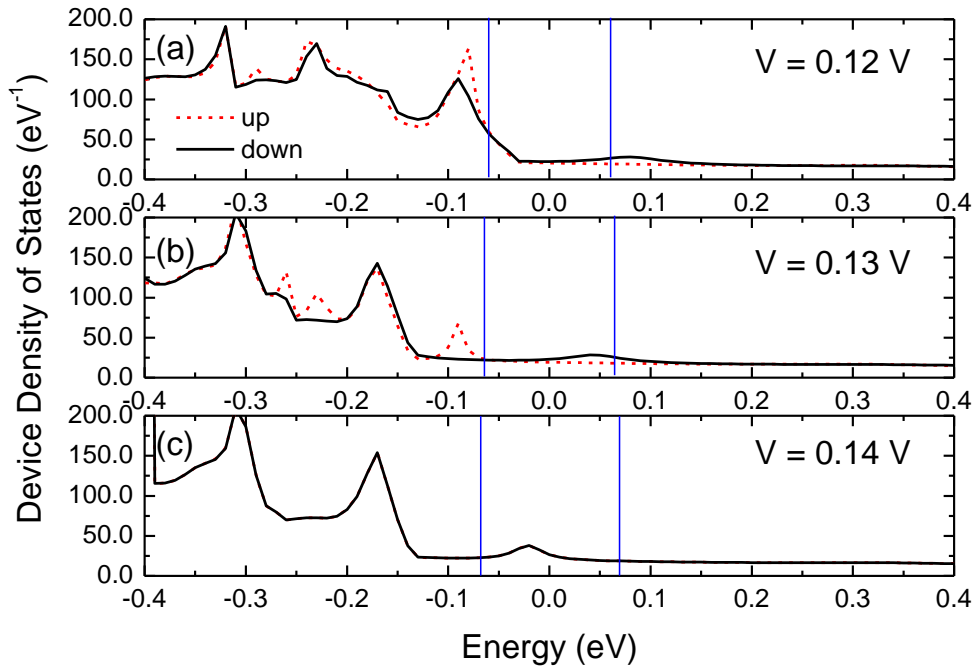


Fig. S12. (a)-(c) The device density of states for the two-probe system of A130Bfree under the biases of 0.12, 0.13 and 0.14 V, respectively.

The coordinates of the optimized A90Bfree, A100Bfree, A110Bfree, A120Bfree and A133Bfree configurations.

A90Bfree

```
# Define elements
```

```
elements = [Palladium, Palladium, Palladium, Palladium, Palladium, Palladium,  
            Palladium, Palladium, Palladium, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron]
```

```
# Define coordinates
```

```
cartesian_coordinates = [[-2.772259515294,    3.944814310597,   -0.811362029537],  
                        [-2.769559887262,    -3.883732430042,    0.859305892855],  
                        [ 0.000101615856,     0.181106089331,   -0.251329574500],  
                        [ 2.772133437740,     3.946653032583,   -0.810182100480],  
                        [ 2.769745821773,    -3.880815859953,    0.859261188450],  
                        [-3.941274182180,     0.036627376764,    0.039446874839],  
                        [-0.000579191058,     3.427648360818,    0.037539437111],  
                        [ 0.003068201480,    -3.312947968803,    0.067592698342],  
                        [ 3.942229600841,     0.039623017223,    0.040339938282],  
                        [-3.224464871366,     1.965097567985,   -0.456889412768],  
                        [ 0.800565555632,    -1.650918125007,   -1.233962286182],  
                        [-0.798824216743,    -1.651773024314,   -1.232963403617],  
                        [ 3.224282338138,     1.966828932523,   -0.456923565877],  
                        [-3.203238180943,    -1.908476305845,    0.465788246393],  
                        [ 0.793465660029,     1.643419363010,    1.272538580311],  
                        [-0.793793549166,     1.642786860599,    1.272854083317],  
                        [ 3.204441591003,    -1.906247775126,    0.465937960785],  
                        [-1.931905936227,    -2.504809404528,   -0.387957796529],  
                        [ 2.065760245766,     0.913030071565,    0.345971601819],  
                        [-1.850055141290,     2.535517099464,    0.303737849968],  
                        [ 2.076550949241,    -0.870385846571,   -0.335259289773],  
                        [-2.075109037139,    -0.872681876657,   -0.335176982207],  
                        [ 1.849389604437,     2.536548506182,    0.303521219983],  
                        [-2.065832916330,     0.911872256916,    0.346507431254],  
                        [ 1.937011180598,    -2.502860041178,   -0.392348543019]]
```

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*Angstrom
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A100Bfree

Define elements

```
elements = [Palladium, Palladium, Palladium, Palladium, Palladium, Palladium,  
            Palladium, Palladium, Palladium, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron]
```

Define coordinates

```
cartesian_coordinates = [[-3.080288350327,    3.983166540838,   -0.630335716564],  
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                        [ 0.000013356201,    0.05804765303 ,   -0.061018124179],  
                        [ 3.080148264156,    3.983289135038,   -0.630395914833],  
                        [ 3.077495357526,   -3.949401057525,    0.637768474237],  
                        [-3.944876040381,    0.020060270691,    0.026975621280],  
                        [-0.000017841979,    3.485586972030,   -0.049586394776],  
                        [ 0.000048947178,   -3.434159342012,    0.058215849428],  
                        [ 3.944875180421,    0.020180371255,    0.026926427119],  
                        [-3.285143384945,    1.962068841745,   -0.436735163013],  
                        [ 0.796017626907,   -1.713350584315,   -1.175275553426],  
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                        [ 3.266697283831,   -1.925739096060,    0.454259490239],  
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                        [-2.060325415123,   -0.904578205622,   -0.257117718330],  
                        [ 1.898090852331,    2.582513989883,    0.247189789614],  
                        [-2.056734952217,    0.939069554059,    0.256666630324],  
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```

*Angstrom

A110Bfree

Define elements

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elements = [Palladium, Palladium, Palladium, Palladium, Palladium, Palladium,  
            Palladium, Palladium, Palladium, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron, Boron,  
            Boron, Boron]
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Define coordinates

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cartesian_coordinates = [[-3.38831718536,      3.975908656872,    -0.442574599492],  
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                        [ 3.388163090572,      3.976042817963,    -0.442602773093],  
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```

*Angstrom

A120Bfree

Define elements

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elements = [Palladium, Palladium, Palladium, Palladium, Palladium, Palladium,  
            Palladium, Palladium, Palladium, Boron, Boron, Boron, Boron, Boron,  
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            Boron, Boron]
```

Define coordinates

```
cartesian_coordinates = [[-3.696346020392,      3.900808778156,    -0.269984726782],  
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                        [ 3.696177916987,        3.900937820919,    -0.269983795333],  
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                        [-3.94918082791 ,         0.016828706808,    0.041823038534],  
                        [-0.000101206912,        3.594849897802,    -0.219891080697],  
                        [ 0.000040022984,      -3.551409292487,    0.194753281313],  
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                        [-3.378949208111,        1.945984655876,    -0.461020431877],  
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                        [-0.798544737834,      -1.853684174337,    -0.961775410358],  
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                        [ 0.798551278108,        1.899837377994,    0.938375437356],  
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                        [ 1.998316335261,        2.696416481063,    0.078349418937],  
                        [-2.054148050127,        1.007716474038,    0.099956965316],  
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```

*Angstrom

A130Bfree

Define elements

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            Boron, Boron]
```

Define coordinates

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cartesian_coordinates = [[-4.004374855425,      3.680991077539,    -0.116991582726],  
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                        [-0.001002428243,      0.022649941808,    0.008648132085],  
                        [ 4.004192743403,      3.679249941097,    -0.117666614311],  
                        [ 4.000743964784,      -3.633921252503,    0.077143376538],  
                        [-3.960539435493,      0.013492113627,    0.102686661305],  
                        [-0.00057577738 ,      3.555291894443,    -0.327265264040],  
                        [-0.000044859043,      -3.495773887098,    0.315283243347],  
                        [ 3.960103826247,      0.013422168676,    0.101403523292],  
                        [-3.363440237947,      1.875193534304,    -0.542791279369],  
                        [ 0.800803451205,      -1.889379962921,    -0.908420572182],  
                        [-0.801682468238,      -1.889776474849,    -0.908640211385],  
                        [ 3.36174347576 ,      1.874322433701,    -0.544886777401],  
                        [-3.307890755583,      -1.874565532328,    0.621582133458],  
                        [ 0.801227345386,      1.947354861502,    0.889853084399],  
                        [-0.80183799122 ,      1.947339120172,    0.890493837136],  
                        [ 3.306234781746,      -1.873200164314,    0.623180626099],  
                        [-2.063426241037,      -2.659000729634,    -0.128498101768],  
                        [ 2.035083040655,      0.994225487298,    0.079939280112],  
                        [-2.056422323169,      2.704481431398,    0.058315951573],  
                        [ 2.029074173217,      -0.955129034581,    -0.020039941231],  
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                        [ 2.055627284290,      2.703910674959,    0.057596915552],  
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                        [ 2.062730343784,      -2.658149204532,    -0.127745443883]]
```

*Angstrom